



LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Energy and Environment Directorate Status Report March 2006

J. C. S. Long

February 23, 2006

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.



Energy and Environment Directorate Status Report

March 2006



**Lawrence Livermore
National Laboratory**

Work performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

Contents

	page
<u>OVERVIEW OF THE ENERGY AND ENVIRONMENT DIRECTORATE</u>	<u>2</u>
BACKGROUND	2
MISSION	3
ORGANIZATION	3
FY06 BUDGET INFORMATION	7
WORKFORCE STATISTICS AND ISSUES	11
PUBLICATIONS	16
SAFETY AND SECURITY	17
ENERGY AND ENVIRONMENT DIRECTORATE VISION STATEMENT	19
<u>DEPARTMENT OVERVIEW</u>	<u>24</u>
COMPUTATIONAL PHYSICS GROUP	26
APPLIED GEOPHYSICS & GEOSPATIAL ANALYSIS GROUP	27
ATMOSPHERIC FLOW, TRANSPORT & HAZARD ASSESSMENT GROUP	28
ENERGY CONVERSION AND STORAGE GROUP	31
NUCLEAR & RISK SCIENCE GROUP	32
CLIMATE/CARBON SCIENCE GROUP	33
GEOCHEMISTRY GROUP	33
CAMS GROUP	35
EXPERIMENTAL GEOPHYSICS GROUP	36
ENVIRONMENTAL SCIENCE GROUP	36
SEISMOLOGY GROUP	37
FLOW AND TRANSPORT GROUP	38
<u>ENERGY AND ENVIRONMENT PROGRAMS</u>	<u>39</u>
NARAC/IMAAC PROGRAM	39
NUCLEAR SYSTEMS SCIENCE AND ENGINEERING PROGRAM	52
EARTH SYSTEMS SCIENCE AND ENGINEERING PROGRAM	53
CENTER FOR ACCELERATOR MASS SPECTROMETRY	63
<u>ACRONYMS</u>	<u>69</u>
<u>APPENDICES</u>	<u>74</u>
APPENDIX A: PUBLICATIONS	74
APPENDIX B: CONTRACT 48 PERFORMANCE OBJECTIVES	75
APPENDIX C: THE ATHENA FRAMEWORK, J.C.S. LONG	86

Overview of the Energy and Environment Directorate

Background

The Energy and Environment Directorate (E&ED) is one of 13 directorates at Lawrence Livermore National Laboratory (LLNL), which is operated by the University of California (UC) for the U.S. Department of Energy's National Nuclear Security Administration (NNSA). We operate in the context of a national security laboratory and focus on meeting major national needs, especially from a long-term perspective.

In the LLNL context, E&ED is a hybrid "program" and "discipline" directorate, combining the program development responsibilities in the national energy and environment arenas to the benefit of the entire Laboratory and also serving as the Laboratory's science base of atmospheric, earth, environmental, and energy science.

This Status Report is part of the annual evaluation process required by the Department of Energy (DOE) as part of its contract with UC. The annual review typically will focus on about one third of the activities and programs of a directorate, so that the entire organization is evaluated over a three-year window. This year's review is focused on the basic science foundations for the directorate and two major program areas in the directorate, with an update from a third program. The programs for review are:

- Earth System Science and Engineering
- Nuclear Systems Science and Engineering
- NARAC/IMAAC update

Major questions to be addressed during this review include:

- (1) Are the programmatic directions appropriate? How can they be improved?
- (2) What actions can E&ED take to ensure success? How well poised for success are the current staff and facilities? What additions are needed?
- (3) What recommendations can be made to the Director and the University?

This Status Report provides background information on the entire directorate including the parts of the directorate that are the focus of this year's review by the Energy and Environment Directorate Review Committee, to be held March 6-9, 2006. The following sections describe the overall directorate structure, the Associate Director's vision for the future, structure and activities of the department and the four major programs, followed by appendices with information about publications, patents, and awards. An additional appendix provides information on the performance objectives used in the performance-based management system that is part of the UC contract to operate LLNL for DOE. The E&E Directorate contributes mainly to performance object 5, "Enhance and nurture a strong science, engineering, and technology base in support of national security strategic objectives." This appendix is included because information from the review committee's

Status Report

report may be included in the LLNL Science and Technology Office's annual report on how LLNL and its directorates meet the performance objectives. We anticipate that the science talks (mainly from the Center for Accelerator Mass Spectrometry) and the science poster session will help the committee assess the E&E Directorate's overall ability to support the scientific needs of LLNL.

Mission

The Energy and Environment Directorate develops, integrates, and applies science and technology to national problems at the nexus of energy, environment, and national security.

Organization

Figure 1-1a shows the current organization of the directorate; Figure 1-1b shows the previous organization from before June 2005 for comparison.

Senior Management Team

Jane C. S. Long continues as the Associate Director, Energy and Environment, a role she has had since November 2004. Norman R. Burkhard is the Principal Deputy Associate Director. Cynthia E. Atkins-Duffin continues as the Deputy Associate Director for Strategic Planning and Resources. Patricia A. Berge became the acting Deputy Associate Director for Operations in November 2005.

Department and Discipline Groups

The line management part of the directorate is the Atmospheric, Earth & Energy Department with 12 groups to focus on nurturing the scientific and technical capabilities of the directorate, growing and developing the workforce, assuring modern equipment and facilities, and investing in the long-term technology base. Norman R. Burkhard is the acting Department Head with John P. Ziagos as Deputy Department Head. The 12 groups include:

- **Seismology**
(Arthur J. Rodgers Jr., Leader)
- **Computational Physics**
(Tarabay H. Antoun, Leader)
- **Energy Conservation and Storage**
(Salvador Aceves, Leader)
- **Nuclear and Risk Science**
(Robert J. Budnitz, Leader)
- **Climate/Carbon Science**
(David C. Bader, Leader)

Status Report

- **Atmospheric Flow, Transport & Hazard Assessment**
(John S. Nasstrom, Leader)
- **Center for Accelerator Mass Spectrometry Staff**
(John P. Knezovich, CAMS Director)
- **Geochemistry**
(Carol J. Bruton, Leader)
- **Experimental Geophysics**
(Frederick J. Ryerson, Leader)
- **Applied Geophysics and Geospatial Analysis**
(Philip E. Harben, Leader)
- **Flow and Transport**
(Andrew Tompson, Leader)
- **Environmental Sciences**
(Gayle A. Pawloski, Leader)

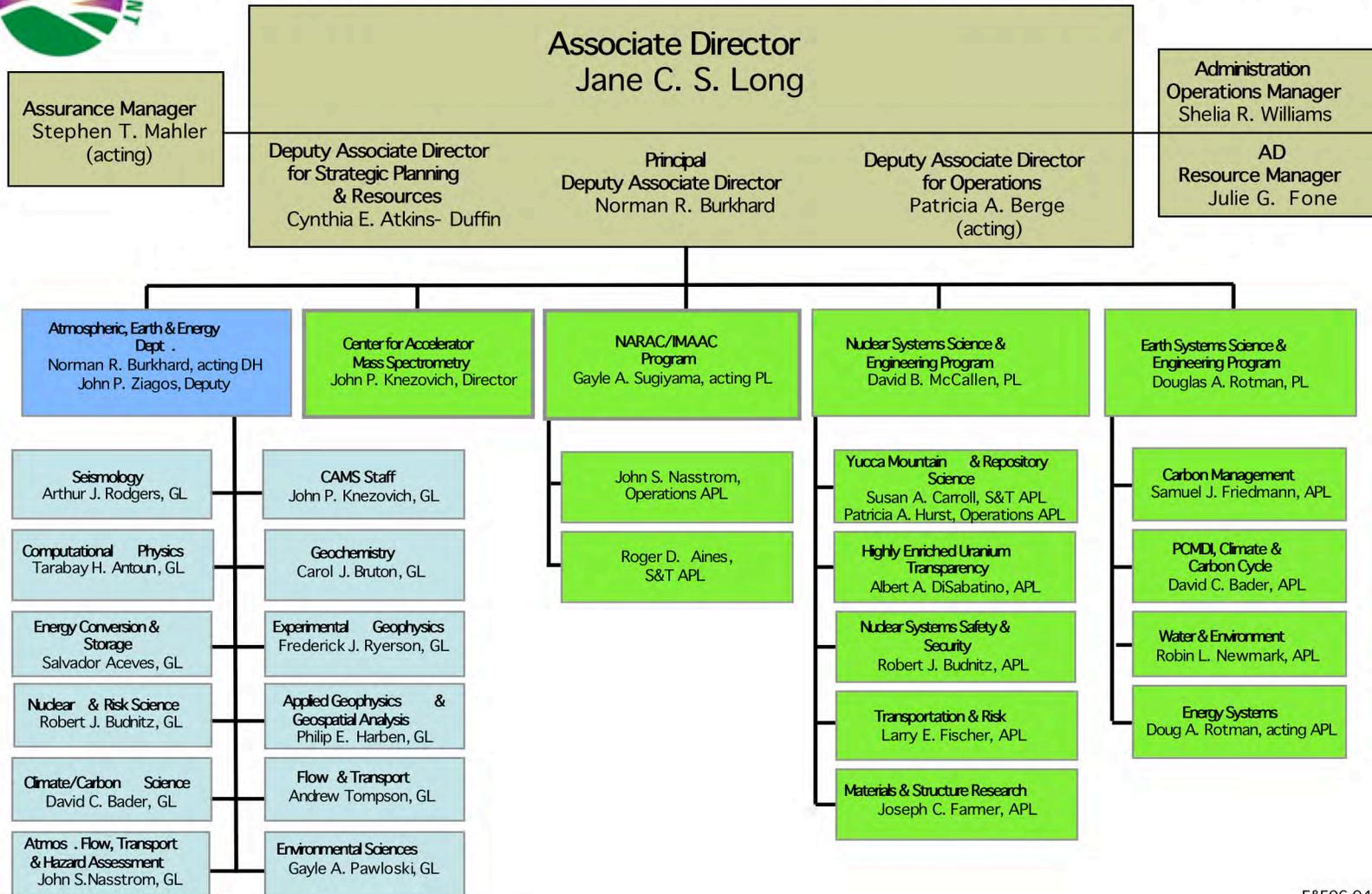
Programs and Center

The three programs and one center focus on the strategic development of new programs and initiatives, capitalizing on Laboratory-wide skills and investments, as well as overseeing the management and execution of externally and internally funded projects. These programs and center include:

- **Earth Systems Science & Engineering Program**
(Douglas A. Rotman, Program Leader; Associate Program Leaders S. Julio Friedmann, David C. Bader, Robin L. Newmark)
- **Nuclear Systems Science & Engineering Program**
(David B. McCallen, Program Leader; Associate Program Leaders Susan A. Carroll, Patricia A. Hurst, Albert A. DiSabatino, Robert J. Budnitz, Larry E. Fischer, Joseph C. Farmer)
- **National Atmospheric Release Advisory Capability/IMAAC Program**
(Gayle A. Sugiyama, acting Program Leader; Associate Program Leaders John S. Nasstrom, Roger D. Aines)
- **Center for Accelerator Mass Spectrometry** (John Knezovich, Director)



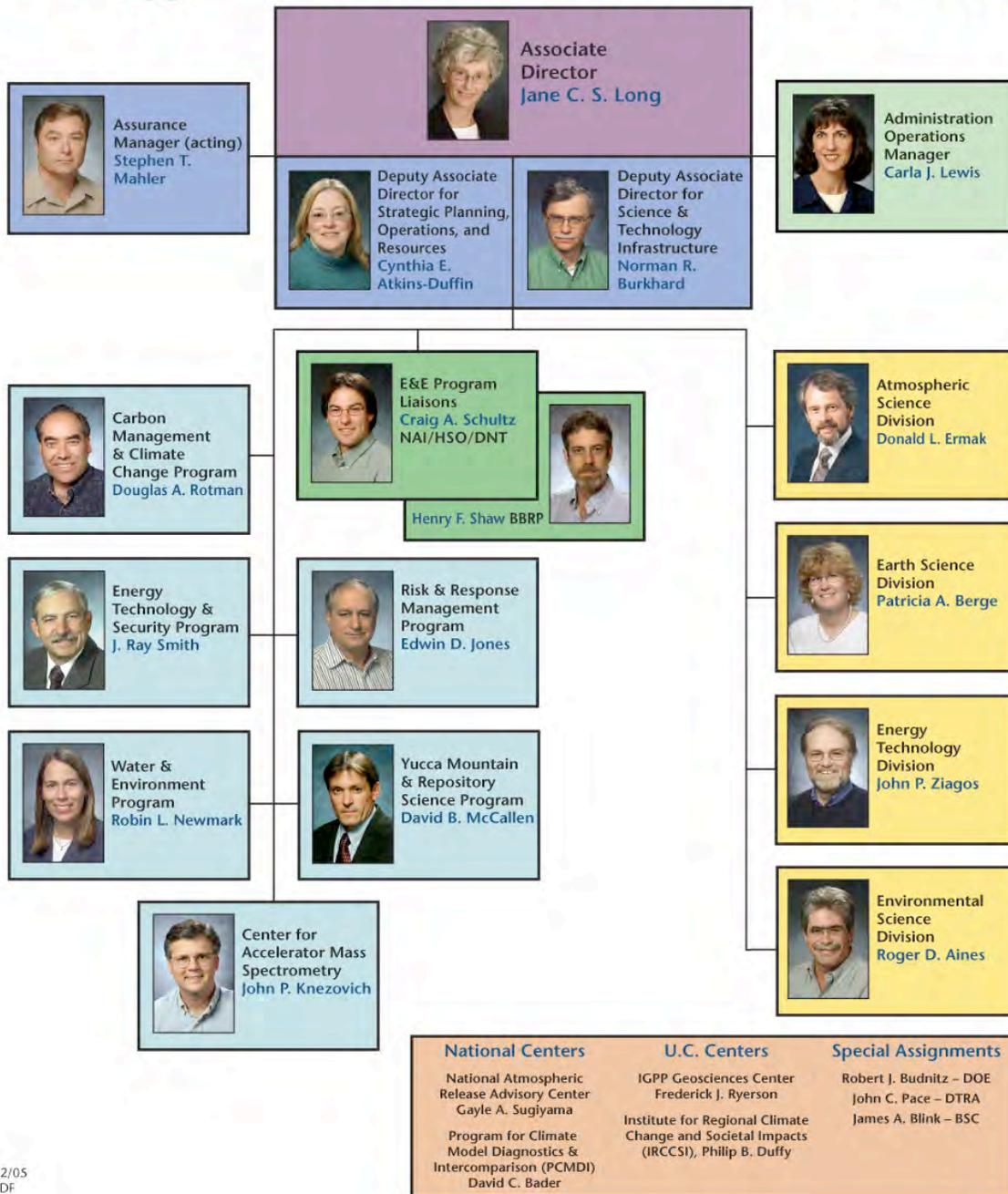
Energy and Environment Directorate



E&E06-046a
1/26/06

Figure 1-1a. The new 2005-2006 Energy and Environment Directorate organization.

Energy and Environment Directorate



02/05
SDF

Figure 1-1b. The Energy and Environment Directorate organization before June 2005.

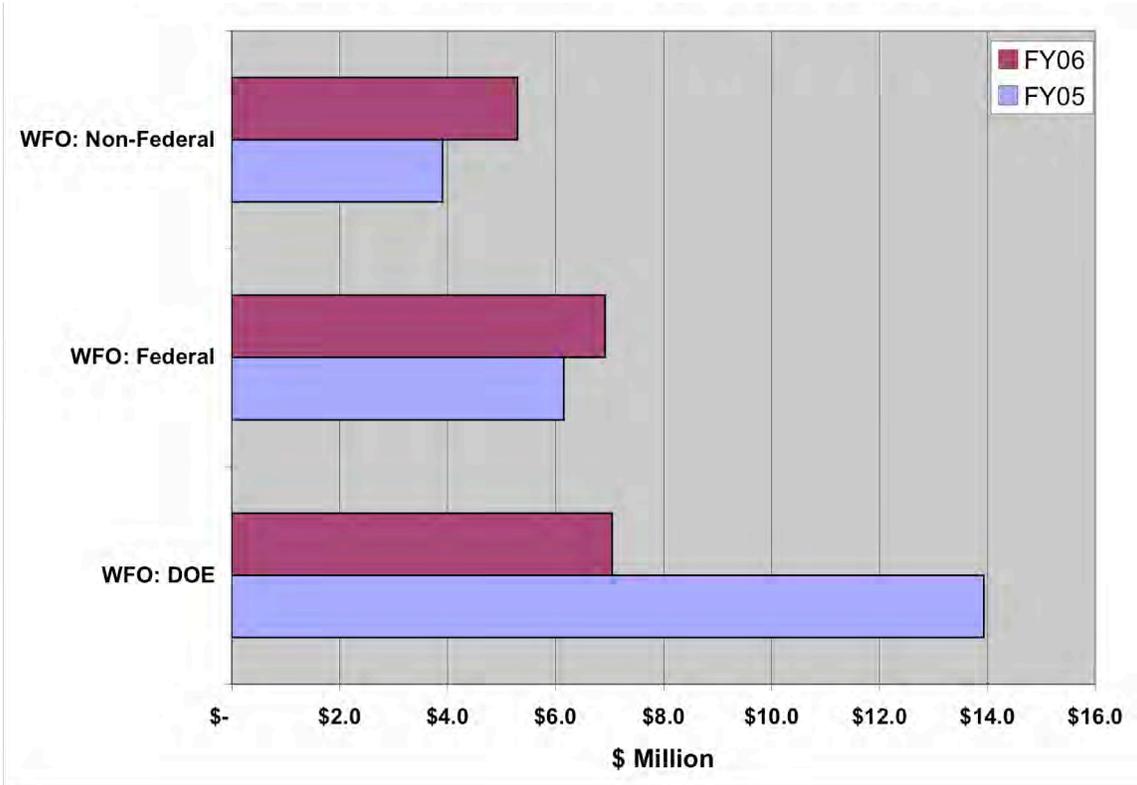
FY06 Budget Information

For FY06, the directorate has about \$79.3 million in estimated costs (budgeted expenditures), which includes about \$66.9 million in direct costs (programs within E&ED) and about \$12.4 million in matrixed-in costs (programs from other directorates managed through E&ED). FY05 actual costs were about \$91.7 million, which included about \$62.6 million in direct costs and about \$29.1 million in matrixed-in costs. Figure 1-2 shows estimated costs by source, Figure 1-3 gives estimated costs by program, and Figure 1-4 lists the directorate's top projects by estimated costs.

This is the same reporting format used last year: estimated current year compared to actuals for the previous year. Last year we overestimated expenditures by about 16% (\$109.3 million estimated, \$91.7 million actual).

There is a \$12 million decrease in estimated costs this year, direct costs increased \$4 million, matrixed-in costs decreased by \$16 million. In FY06 we changed the way in which we track our matrixed-in funding, thus resulting in a \$9 million reduction. The Security & Protection Program also moved to the Security & Environmental Protection Directorate resulting in a decrease of \$8 million. FY06 funding has been coming in late this year due to the continuing resolution. This may result in our once again spending below our current estimate, for a net decrease in overall E&ED program activity.

All budget figures are based on actual expenditures, rather than on funding received. This avoids uncertainty associated with carryover, since many of our programs receive funding in mid-year.



**E&ED FY06 Work for Others, Estimated Costs (\$19.2M)
compared to FY05**

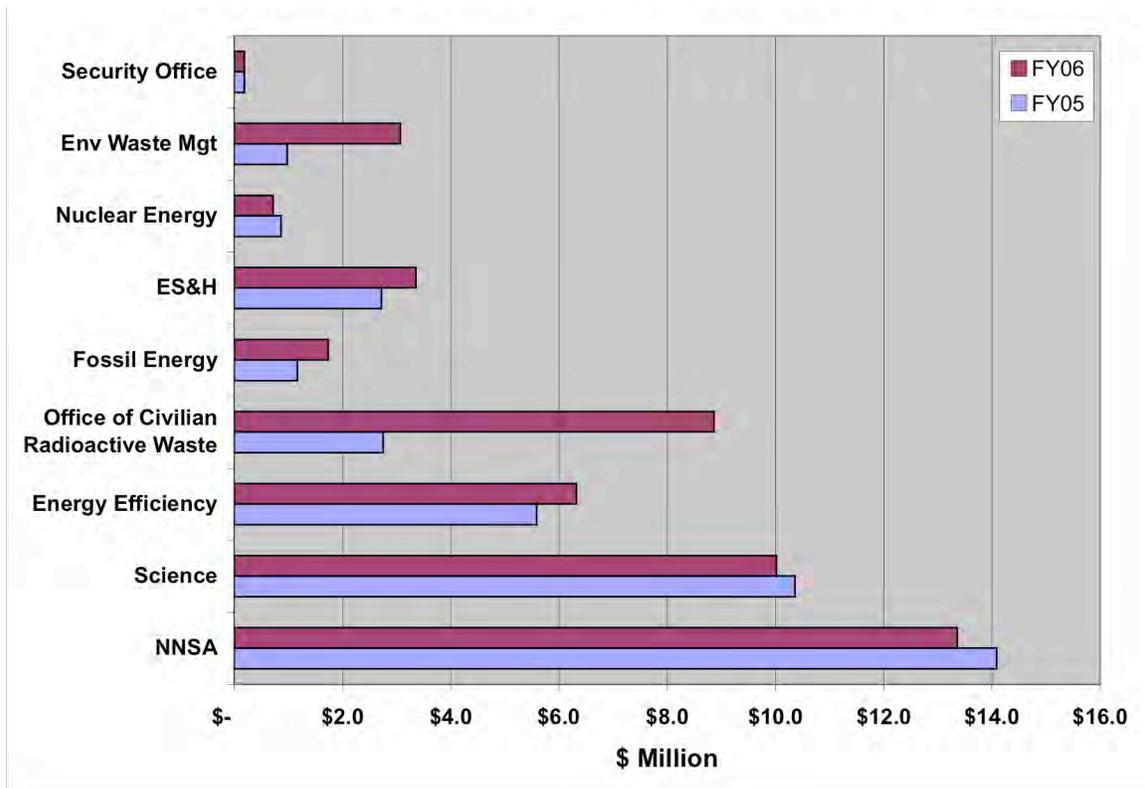


Figure 1-2. E&ED has total estimated costs (budgeted expenditures) of about \$79.3 million, which comes from a variety of sources: (a) DOE and NNSA, (b) work for others, and (c) matrixed-in and internal sources. (Data as of January 28, 2006.)

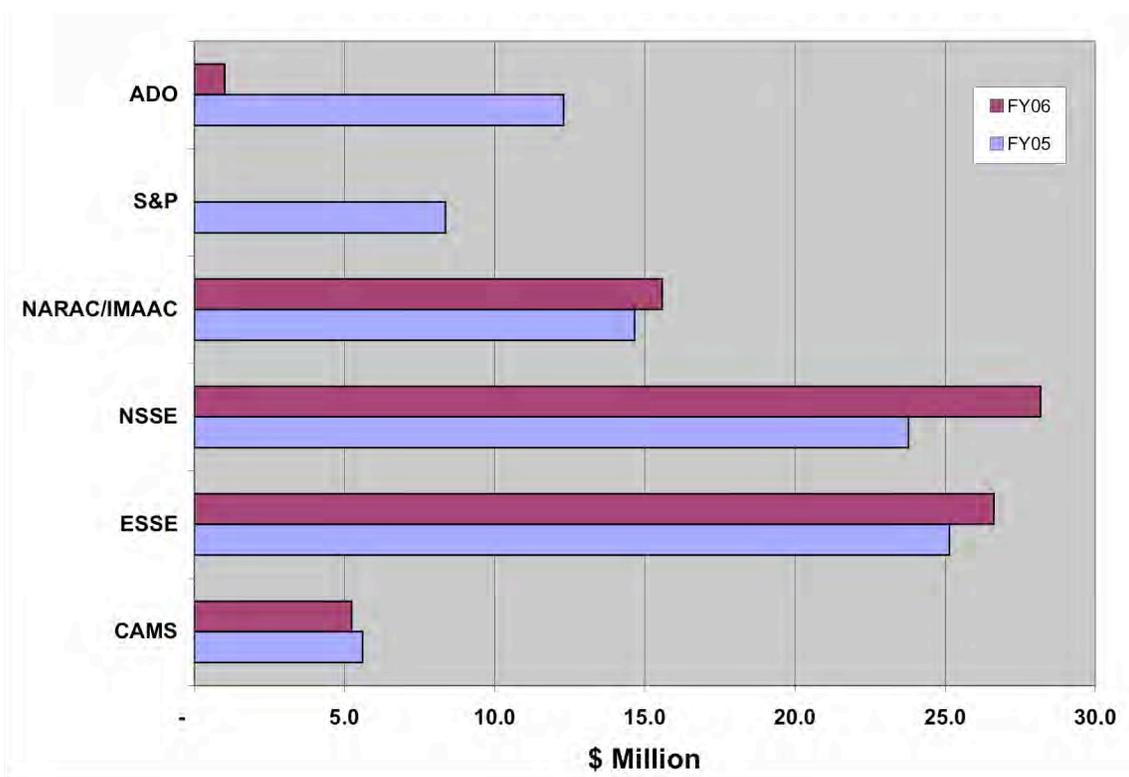


Figure 1-3. Total FY06 Estimated Costs by Program Compared to FY05 Actual Costs. This chart does not include G&A costs. In addition to the matrixed-in programs managed by E&ED, the directorate provides about 90 FTEs of support to other LLNL programs. (Data as of January 28, 2006)

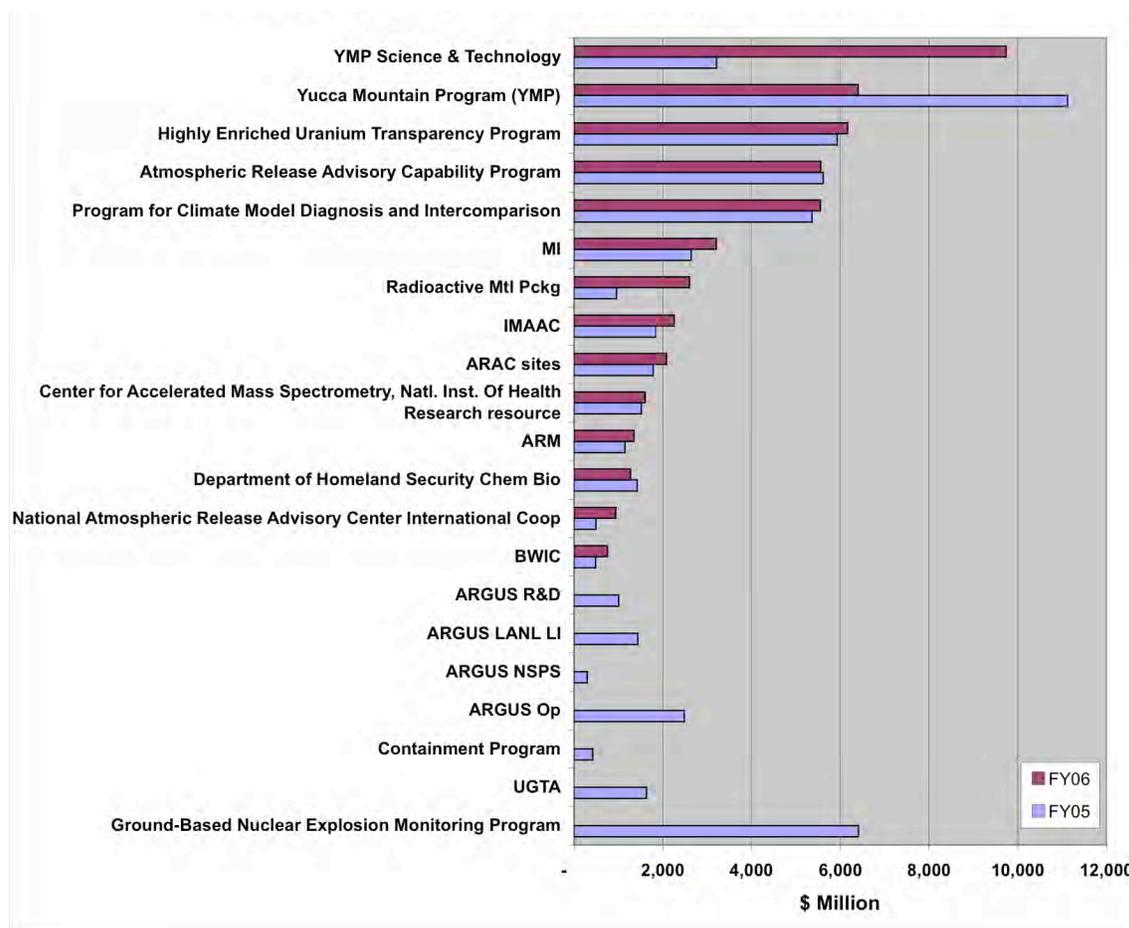


Figure 1-4. E&ED Top Projects by Estimated Costs FY06 Compared to FY05 (Data as of January 28, 2006)

Workforce Statistics and Issues

The directorate has a strong scientific and technical staff, representing a broad range of skills. The professional stature of our employees is underscored by the information included in the appendix.

LLNL operates with a matrix system, which means that some of our scientists and engineers perform work for E&ED programs and some are matrixed to other directorates. In turn, we rely on staff from other Laboratory directorates to perform work in some of our programs. Chart A shows the source of personnel supporting E&ED-led programs in FY06, compared to FY05, and also the number of E&ED full-time-equivalent (FTE) employees supporting various LLNL directorates (including the E&E Directorate) in FY06, compared to FY05.)

Chart B shows the distribution of E&ED employees by broad job category. Chart C shows the job category distribution of employees matrixed into E&ED from other

directorates. There are 157.3 FTEs of E&ED personnel working in our own programs and 118 FTEs charging E&ED accounts. Our programs support a total of 275 FTEs. The decline in matrixed FTEs appears to reflect both the major cutbacks in the Yucca Mountain Program and late delivery of funding this year.

Chart A Employees Matrixed into E&ED Programs FY06 by Job Category

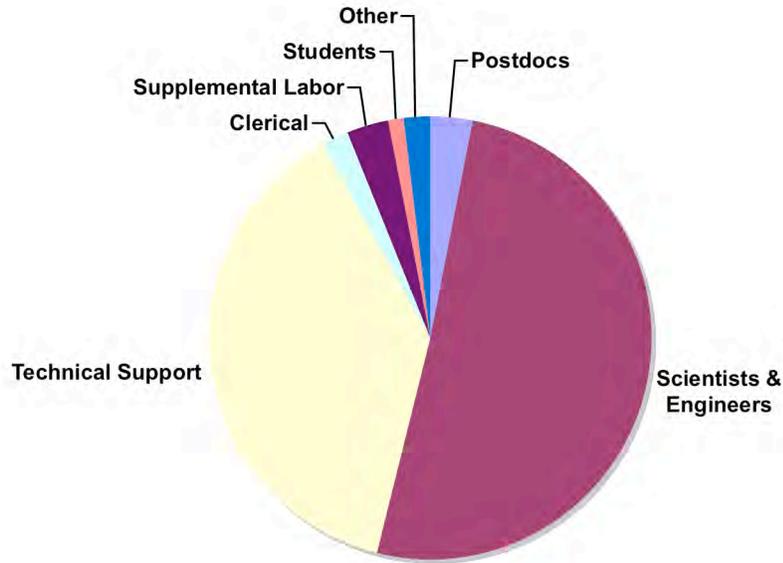
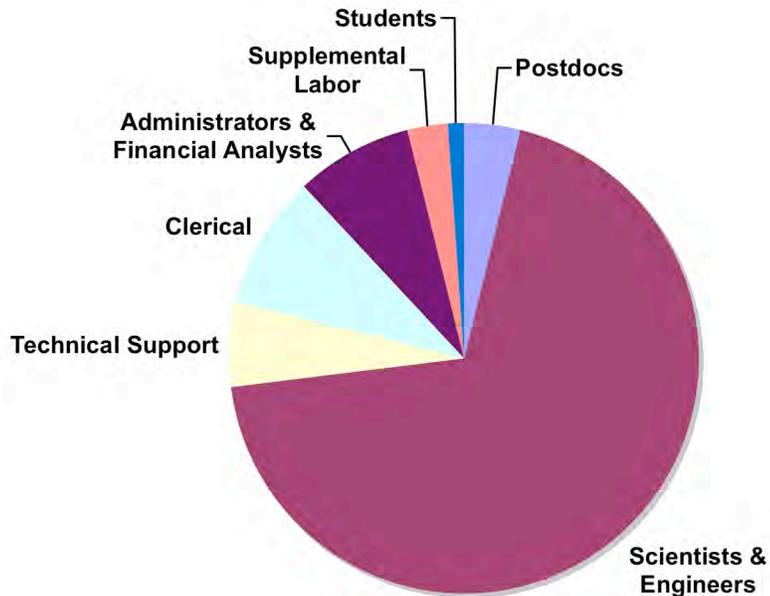
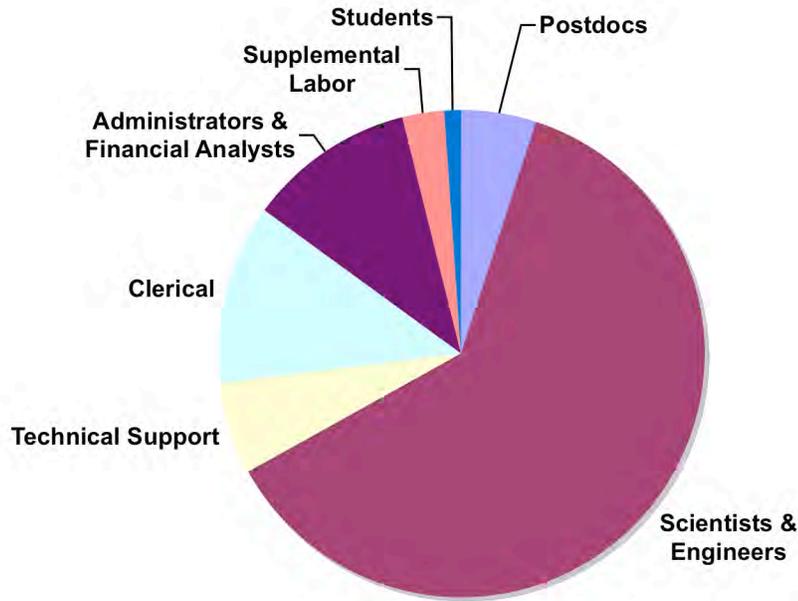


Chart B All E&ED Employees Charging All LLNL Accounts Total FTEs: 246.09



**Chart C E&ED Employees Charging E&E Accounts
by Job Category Total FTEs: 157.3**



Workforce Development Efforts

The E&E Directorate, like the Laboratory as a whole, has a highly experienced but aging workforce and faces the need to replace those who are retiring or who leave for other purposes. Strategic hiring has been a focus for the directorate in the past year. We are focused on ways to attract newer, younger employees—especially those with the particular skills needed for future work. We are working to implement better channels for career development and ways to enhance the work experience at LLNL, such as alternative work hours and maintaining a competitive reward system.

For this study employees have been grouped into three retirement sets:										
	early career (less than 35 years with less than 10 years of service)									
	retirement eligible (meet the minimum 50 years and 5 years service requirements)									
	more likely to retire (over 55 years and 10 plus years service)									
	most likely to retire (over 60 years and 20 plus years service)									
Series	Age Cohorts	0-4	9-May	14-Oct	15-19	20-24	25-29	30-34	35+	Total
200s	<20									
	20-24									
	25-29									
	30-34	1	2	1						4
	35-39	1	3	4						8
	40-44	3	8	10	2					23
	45-49	2	1	9	11	6	1			30
	50-54		2	3	5	7	9	2		28
	55-59		1	5	7	8	8	6		35
	60-64				1	1	3	3	3	11
	65+			1	1			1		3
200s Total		7	17	33	27	22	21	12	3	142

E&ED's scientists and engineers by age and years of service showing those in early and late career stages (as of 10/1/05).

Changes in E&ED Staffing FY05 to Present

	Scientists and Engineers	Technical and Administrative
New hires	6 Postdocs	1 Flex Term
Retirement	11	7
Moved elsewhere at LLNL	9	10
Left LLNL	9	7
Transferred in from LLNL	1	1

Postdoctoral Program

The Energy and Environment Directorate is committed to maintaining a strong postdoctoral program. We believe that an active postdoctoral program is essential for maintaining the technical vitality of directorate organizations and expands their research horizons. In particular, a postdoctoral program contributes to the health of the Energy and Environment disciplines at LLNL by:

- Ensuring an influx of new ideas, energy and enthusiasm.

- Contributing to the Laboratory's education mission.
- Enhancing the productivity of the organizations and their programs.
- Renewing old contacts and establishing new contacts with academic and industrial communities.
- Establishing contacts with future employers of our postdoctoral employees.
- Fostering new collaborative programs, enhancing recruiting for E&ED and LLNL as a whole, and improving our directorate's visibility and image.

E&ED currently has a population of approximately 13 postdocs and we expect to have as many as 15 by the end of this calendar year. To ensure that the objectives listed above are met and that all parties have a rewarding experience as our postdoc population continues to grow, the Directorate created an internal Postdoctoral Committee in June 2003. The committee continues to meet in 2006.

The current chair of the E&ED Postdoc Committee, Michaele Kashgarian, also serves as the E&ED representative to the LLNL Lab wide Postdoc Advisory Council (PDAC) and is contributing to the design of the external LLNL.gov web page used for recruiting new postdocs to LLNL. The PDAC developed an agreement with the National Academy of Sciences to begin a National Research Council postdoc program at LLNL, which is expected to increase the number of postdocs across the lab as a whole.

The E&ED Postdoc Committee continues to hold brown bag lunches on various topics for postdocs to foster communication and provide E&ED-specific informal training to supplement the lab-wide postdoctoral orientation sessions held each fall. In addition to brown bag Q&A sessions with E&ED upper management, we have had briefings from the Foreign National Office, Laboratory Science and Technology Office, and an E&ED Ombudsman representative as well as informal social gatherings. The E&ED Postdoc Committee also maintains a web site (<http://eed-r.llnl.gov/postdoc/>), which serves as a bulletin board and information resource.

The main focus of the committee's activities over the past two years has been to improve the relationships between research mentors and postdocs. We have drafted a set of guidelines (available on request) which we hope will help research mentors and postdocs work together to craft a productive research and training plan during their time at LLNL and to help postdocs achieve their career goals.

The committee also coordinated our third annual postdoctoral poster symposium in February 2006, in which all but one of the postdocs in the directorate participated. (Some of those posters will be included in the directorate review.) Directorate awards were given for the best posters. E&ED postdocs have been featured speakers in directorate and program seminars. In 2006 the committee plans to continue our successful brown bag series for postdocs and continue to implement the mentoring guidelines document.

Support of Conferences and Professional Societies

The E&E Directorate values the leadership roles that our scientific staff fills for the scientific community, because the quality and recognition of our science is a key component of recruitment, staff careers, and our success. For these reasons, the directorate has established a program to encourage our scientific staff to become more involved in running relevant professional societies. Susan Carroll, who has a long service record with the American Chemical Society, manages this program.

The American Geophysical Union (AGU) is an important society to the directorate because it is an inclusive geophysical organization representing atmospheric, hydrologic, solid earth, ocean and space sciences. Last year the directorate supported associate and deputy editors of three AGU journals, five AGU committee members, and helped organize an AGU Chapman Conference. This year, we are also supporting a co-chair of the AGU sponsored *Western Pacific Geophysics Meeting* in Beijing China.

In addition to supporting a single society that cuts across the directorate, we also think it is important that we have leadership roles in societies that reflect the diversity of research conducted in the directorate. We have strong leadership roles in the American Meteorological Society, for which the directorate supported the efforts of the chair for a special symposium on Global Change and Climate Variations and members of the Climate Variability and Change committee. One of our employees is the president of the American Rock Mechanics Association and vice-president of the International Society for Rock Mechanics, and several staff hold editorial roles for major journals. Our support also extended to the organization of three major conferences: the *International Conference on Accelerator Mass Spectrometry*, the *51st Radiobioassay and Radiochemical Measurements Conference*, and the *International Symposium on Systems and Human Science for Safety, Security, and Reliability*.

Publications

Appendix A lists the publications by E&ED employees in 2005, and the following table summarizes them by category.

E&ED publications, calendar years 2005, 2004, and 2003.			
	CY2005	CY2004	CY2003
Number of papers published in peer-reviewed journals	xx	77	88
Number of journal articles submitted but not yet published	xx	120	85
Number of books or book sections published	xx	7	3
Number of technical or programmatic reports	xx	128	101
TOTAL PUBLICATIONS	xxx	332	277

Safety and Security

Environmental Safety and Health (ES&H) Performance

The health, safety, and environmental performance of E&ED is a directorate priority. Integrated Safety Management is now fully incorporated into our scientific and operational practices. E&ED continues to take a proactive approach to its ES&H program, incorporating a strong ES&H philosophy into all aspects of work activities. E&ED's ES&H support system—consisting of the directorate's AD Facility Manager, ES&H Operations Manager, Facility Points of Contact, Subject Matter Experts in Hazards Control's ES&H Team 4, and administrative support—continues to function in a coordinated fashion, with good cross-communication. ES&H support elements receive full management support.

Our recordable injury/illness record remains low for the reporting period, as is our accident/injury cost index. The accident/injury cost index for E&ED indicates the approximate dollar loss of all work-related injuries and illnesses per 100 hours worked. E&ED had a low "day away: restricted/transferred" (DART) rate for calendar year 2005. (The "lost days" are the number of calendar days [consecutive or not], beyond the day of injury or onset of illness, that the employee was unable to work because of a work-related injury or illness). As Table 1-4 shows, our most recent four years are favorable compared to our eight-year record. However, the number of employees and cases increased, although the severity and DART rate decreased in CY2005.

E&ED conducts numerous formal and informal assessments of its various operations and infrastructure issues throughout the year in accordance with the previously approved self-assessment plan. The directorate uses these opportunities for managers, supervisors, workers, ES&H/Facility Support Team staff, and ES&H Team members to work collectively on ES&H awareness issues, enhance communication and support, and help to ensure ES&H requirements are being met. Noted deficiencies are entered into the Issues Tracking System (the institutional deficiency-tracking system).

Cumulative stress and repetitive motion injuries, such as carpal tunnel syndrome, continue to be addressed through a program of comprehensive education and awareness and through individual workstation analysis. The directorate requirement that every E&ED employee take Web-based ergonomic training (so that individual ergonomic evaluations can be the most effective) is believed to strongly contribute to a reduced rate of cumulative injuries.

Table 1-4. Injury data reported in calendar years 1998 through 2005

Calendar year	No. of employees with recordable injuries	Recordable injury/illness case rate	DART rate	Severity rate	Cost index
1998	13	3.73	1.43	58.54	100.44
1999	11	3.45	1.26	108.26	43.84
2000	8	2.76	.34	23.45	7.45
2001	7	2.6	1.11	9.65	5.64
2002	4	1.41	0.35	1.41	2.12
2003	2	0.7	0.35	.35	0.87
2004	4	1.48	0.37	2.6	2.78
2005	5	2.12	0.00	0.00	2.12

Security Performance

E&ED continued to deploy Integrated Safeguards and Security Management (ISSM) in the directorate during the reporting period, cooperating with LLNL-wide implementation of ISSM and aligning our approach to security with new LLNL guidance. Appropriate security remains paramount within our organizations as we update security strategies to be consistent with ISSM. E&ED's security objective is to protect LLNL assets using a security approach that is compliant, effective and sensible. We continue to ensure that security roles and responsibilities are clear from the Associate Director through the management chain to the worker. We use cross-directorate forums (The Operations Security Council, the Directorate Safeguards and Security Officers group) to incorporate best practices and use security self-assessments to indicate improvement areas.

E&ED's security performance needs improvement. In 2005 we had four reportable incidents that involved two E&ED employees and two CMS employees matrixed to E&ED. Although all four incidents were determined to have low impact, they are incidents that in combination and over time could pose a long-term threat to DOE security interests by adversely impacting the level of security awareness and program responsiveness. Three of the four were determined to be security infractions. This represents an increase from previous years since we typically had two or fewer infractions in 2001 through 2004. LLNL had 76 infractions in 2005.

Energy and Environment Directorate Vision Statement

Jane C. S. Long, Associate Director

Over the past year, I have focused on four major activities:

1. Reorganizing and focusing the directorate
2. Obtaining internal strategic funds and conducting strategic initiatives
3. Hiring key staff
4. Maintaining funding from DOE and other agencies

Reorganization

Shortly after the DRC met last spring, we began an effort to streamline and focus the directorate. The issues we faced included top-heavy, costly management, declining budgets and a structure that was in places redundant, confusing, costly and unfocussed. The reorganization was conducted through a series of working meetings that collected information and input. A draft version was circulated for comment and then a final version was put in place in May of 2005. The old organization chart and our new one are shown in Figures 1-1a and 1-1b.

The new organization maintained some of the essential qualities of a “hybrid” directorate. That is, we are both a program directorate and a disciplinary directorate. On the disciplinary side, we previously had four divisions each divided into about four to ten groups. We eliminated the division structure and created one large department with 12 disciplinary groups. The group leaders now all report to the Principal Deputy AD, Norm Burkhard. This flattened our structure and eliminated boundaries between divisions. It also gave the group leader position more responsibility. Each group now has about 10 to 25 people. The groups are quite heterogeneous. In some, all are working on the same program (e.g. Climate/Carbon Science Group, NARAC/IMAAC Program). In others, the scientists are working on many different projects (e.g., Geochemistry Group). In some groups, the scientists work on our projects, and some are entirely employed by other directorates (e.g., Seismology Group supports the Ground-based Nuclear Explosion Monitoring program funded out of the NAI Directorate). In one case the group is literally the same as the program (CAMS). The groups provide our personnel supervisory structure. This is not a “perfect” structure; it is pragmatic and aimed to eliminate a layer of management while maintaining the benefits of separation between personnel management and program management offered by the matrix system.

We then refocused the programmatic side of the house into four areas. The purpose was to provide a systems-oriented structure. First, we established the Earth Systems Science and Engineering Program (ESSE). This program includes all of our work on climate, water, energy and carbon sequestration. The program is headed by Doug Rotman and now is able to integrate solutions to the climate-energy-water problems. Doug is doing a fantastic job coordinating this group that has never before worked together. The energy program now has a clear focus on energy systems that meet our future energy services

demand, but also respond to the climate problem. The climate scientists now benefit from an increased interaction with energy systems engineers. The connection between energy and water is better represented, and carbon capture and storage is placed appropriately in the climate-energy arena. Four sub-programs include climate (Dave Bader), water and environment (Robin Newmark), carbon capture and storage (S. Julio Friedmann) and energy systems (Doug Rotman, acting). This last position has been posted and we are conducting an extensive search for a candidate. Although the need for the focus of this program is clear, Federal funding has been problematic. Consequently, the strategy we have is to develop our ideas about solutions to the real problems as we understand them, engage the state for funding and support, and continue to work with DOE hoping for continued support from the CCSP, CCTP and perhaps a new Energy/Water Nexus program.

Next, we established the Nuclear Systems Science and Engineering Program. Although this could have been part of ESSE, it represents such a large and complex problem in and of itself, that we made it separate. The NSSE brings together our work on Yucca Mountain, reactors and nuclear fuel cycles. Dave McCallen is heading this program and is providing leadership to the national nuclear power initiative headed by Vic Reis called the Global Nuclear Energy Partnership (GNEP). We have forged cooperation with the UC Berkeley Nuclear Engineering Department. We now have a program that looks at nuclear power as a cradle-to-grave problem and can focus on what it will take to make nuclear power an option for our energy future, including safety, security, public perception, waste and economics.

Third, we established the NARAC/IMAAC Program. This major program had formerly been submerged in the Risk and Response Program. However, it is perhaps one of the most visible programs in the directorate and the Lab for that matter. The future of the program rests on landing the IMAAC project from the DHS and required a direct communication with the AD, as well as strong communication with the AD for NAI. Gayle Sugiyama is heading this program along with two deputies: one for operations (John Nasstrom) and a new one for science and technology (Roger Aines). The review process for awarding the IMAAC has recently begun and so far is going quite well. The strategy includes serving as a hub for other organizations working on atmospheric release, providing an operational facility in the context of a research organization capable of responding to unexpected situations, and developing a plan for scaling up operations on an emergency basis to laboratory super-computers and to an expanded work-force.

Finally, CAMS was elevated from a sub-program within the Environmental Research Program to a stand-alone program. CAMS is a unique facility that serves E&ED missions as well as missions in chemistry and materials, weapons, biology, medicine and national security. CAMS is also one of the most visible parts of the directorate and laboratory and merits the status of reporting directly to the AD. CAMS, under the excellent leadership of John Knezovich, continues its success in basic and applied research and is one of the jewels of the laboratory.

So far, we seem to be doing well with this structure. However, it isn't perfect. The major problem has been that the groups have to act like smaller programs – they aren't perfectly "disciplinary". The group leaders and many of the scientists still have to be entrepreneurial about obtaining research funds. Consequently we bridge between the group leaders and the program leaders in an ad hoc manner. I meet with group leaders about once a month, top-level program leaders together once a month (on an individual basis we meet much more frequently) and with program and associate program leaders once a month. To bridge the gap, we will now invite group leaders to the latter meeting. I expect this will be of interest to about half of them. Program leaders are asked to coordinate directly with those groups who relate most strongly to their programs. As well, I meet with directorate leaders in national security projects once a month. The structure has saved us over a million dollars per year. Given the increase in lab overhead and declining budgets, this has allowed us to keep directorate overheads nearly level.

Obtaining strategic funds

Our Deputy Director for Science and Technology, Cherry Murray established a strategic planning effort, called the Aurora Project that started in the spring of 2005 and reached first action in the fall. This effort involved four lab-wide committees: science and technology, mission, workforce and operations. I co-chaired the missions committee that met nearly every week. Each committee sponsored a number of proposals for strategic funds. These were presented in an off-site meeting in July. Our proposal for an initiative in energy ranked second among all of the projects presented at the offsite. We also presented initiatives in nuclear energy and in developing a stronger relationship with the state of California and UC. From July until about November, decisions about funding were made in the context of expected budget cuts at the lab and the need to trim overhead funding in order to fund new projects. In the end our energy initiative was combined with the California initiative and funded for \$1.5M and the nuclear initiative was funded for \$600K.

The combined energy/California project falls under our climate and energy initiative, which we have called the Athena Action Plan. A paper I wrote for the L20 Energy Security Workshop held at Stanford University in October 2005 about Athena is attached.

We have organized our efforts in three areas:

Understand the problem and predict outcomes: The interaction of human behavior with the Earth's natural systems is at the heart of the climate and energy problem. We need to develop the scientific basis and capacity to understand how natural systems will behave in concert with human activity. *How* will temperature rise, and *what* in turn will the rise in temperature cause? At this time we find that climate change models are able to predict with some accuracy (within a few degrees) the mean temperature of the Earth if they know the level of greenhouse gases in the atmosphere. However, in the last hundred years, nearly half of the emitted CO₂ has ended up dissolved in the ocean, not in the atmosphere. We don't know how long this will continue and consequently, we don't know how various emission scenarios that might be agreed on among nations will result in CO₂ levels in the atmosphere. Thus, we do not know with much accuracy at all

how emission scenarios will increase temperature. What we need is a major international research program on the fate and cycling of carbon in the Earth's atmosphere, hydrosphere and biosphere. We need to know where the carbon will go and how long it will stay there. Aurora funds will support our initiative leaders in the carbon cycle.

frequent droughts, and increasing water demand, extreme events of deadly consequence such as heat waves, storms, floods and forest fires, disruptions to agriculture, sea level rise, coastal erosion, melting of the permafrost, decreased pH and warming of the oceans leading to ecological damage, degraded air quality and migration of disease vectors, ecological damage due to habitat loss will all be more likely. We need the foresight to prepare for and adapt to changes in our environment caused by global climate change. If policy makers are to deal with these, they need accurate estimates of increased risk due to climate change, and their costs, a wide range of technical and policy tools for dealing with the risks estimates of the cost of mitigation. At this point in time we have no coherent national program to address adaptation. We are not prepared for disasters that will become more frequent and more severe. We don't know how vulnerable we are and we don't have the information needed to make societal choices like raising the levees or building new water storage or purification systems. We need a new national focus on adaptation and perhaps even more importantly, we need to focus on adaptation in the developing world where there are not the resources. It is time to define a climate change adaptation program. A significant part of this program should be conducted on a regional basis. Problems with the melting of permafrost in the arctic of Alaska will be quite different than the inundation of New Orleans or the loss of water supply due to melting glaciers. Aurora funds will support hiring a regional climate scientist and to support coordination with the State of California on regional climate and adaptation technology.

Develop a clean energy system for the world: We need to develop energy technologies that do not cause global climate change and are, as well, not a threat to our security or economic well-being. Our analysis shows that this problem is huge. We have to double the amount of energy we have available in the next 50 years and we have to essentially reduce emissions to zero. We need to throw everything we have at the problem – and more. We need a portfolio of solutions that will enable us to provide clean energy to all the peoples of the world. We need a five-part energy program. The first part is better energy systems analysis leading to better energy policy. The second key issue is energy conservation and efficiency. It is possible to maintain the same standard of living and use much less energy than we do. The third is carbon capture and storage. There is probably no way to have enough energy to meet demand without using fossil fuels, and worse, using coal. The fourth is improved energy transmission, storage and co-generation. Finally, we need to promote energy with no carbon emissions. Aurora funds are supporting the formation of the California Energy Modeling Consortium between LLNL, LBNL, Stanford and UC Berkeley. This group will submit a proposal for moving energy system modeling forward as a group effort.

Aurora money is also supporting the GNEP program. Under the leadership of Dave McCallen, we have been involved in running the first GNEP workshop and in preparing the plans for future work in nuclear energy (see NSSE summary later in this report).

Hiring Key Staff

A critical problem for us now is hiring into key positions for this structure. There are two key positions: energy and regional climate. Ray Smith stepped down from the Energy lead in October. We have been searching for a replacement. Also, given the focus on energy systems modeling, we need to find someone who is experienced in this area. We have posted two positions, one to lead our energy technology program, including energy systems modeling and one to lead the modeling, and are considering external as well as internal candidates. The other position is in regional climate modeling. The focus on California and a focus on developing adaptation technology and risk assessment mean that we need a lead in regional climate. We are looking for a mid-career scientist to lead this program.

Maintaining DOE/ Federal funding

ESSE, NSSE and NARAC/IMAAC are all involved in major strategic efforts on the national scale. Julio Friedmann and I represent the laboratory on the Laboratory Working Group that is chartered to give Under Secretary Garman advice about how to choose research directions. A large number of our scientists have participated in the various sub-committees. Currently, I chair the long-term evaluation committee. We have been developing a recommendation to DOE that they revitalize energy policy analysis as a way to illuminate energy goals. It is difficult to evaluate a research portfolio with out explicit goals. If adopted this recommendation would strengthen the CCTP and hopefully provide more avenues for research.

Dave McCallen is leading our participation in the Global Nuclear Energy Program that has been highlighted in the media of late. We believe that our long-term participation will be in the area of improving the economics through modern safety design (computationally intensive), siting, managing nuclear waste, and in high-temperature material science (also computationally intensive).

Finally, as mentioned above, we are deeply involved in competing for IMAAC as a permanent program. As of April 2004, we are the acting IMAAC for DHS. The review process began in February with the visit of a consulting committee. The major problem we face is a lack of clear understanding of how DHS will make a decision.

Department Overview

During the summer of 2005, the Energy & Environment Directorate's divisions were reorganized into a new Atmospheric, Earth, and Energy Sciences Department with 12 discipline groups. This reorganization was intended to streamline the line management organizational structure, reduce overhead costs, and align the directorate's discipline and technical base and capabilities with E&ED's mission and strategic planning areas (i.e., earth system science, nuclear energy, and national security). Streamlining the management structure was intended to empower group leaders by giving them authority to match the responsibilities of the group leader role, and direct access to overhead funds so that they would have the required resources to carry out their responsibilities. The realignment was done to ensure the science and technical environment in E&ED is robust and poised for current and future activities. The 12 group leaders coordinate capabilities of the discipline staff with needs of programs inside and outside the directorate.

The vision for the new department is to have the department be an outstanding resource for the Lab and the nation, for basic and applied research in atmospheric, earth, environmental, and energy sciences relevant to national security, energy, and environmental programs. Science must be outstanding, within a framework of outstanding business practices, safety, and security. Achieving this vision requires attention to the following:

- People
 - Supporting and encouraging E&E Directorate's outstanding staff
 - Recruiting outstanding postdocs and strategic hires to replace retiring staff
 - Maintaining and expanding technical expertise in core discipline areas
 - Succession planning as staff retire
- Funds
 - Stabilizing and increasing programmatic funding, particularly in areas of interest to the AD (energy and environment) and areas likely to have growing budgets (programs in NAI Directorate and Homeland Security)
- Strong Relationships with Others
 - Enhancing interdisciplinary collaborations and programmatic ties between E&E Directorate groups and between E&ED and other directorates at LLNL
 - Strengthening ties to scientific societies and relationships with the research community outside LLNL and DOE
- Equipment
 - Upgrading experimental and computational infrastructure.

The department has approximately 200 scientists, engineers, and technical personnel. Descriptions of each of the 12 groups are provided below, including discipline expertise

and composition of each group, experimental facilities, computational codes or other critical tech base assets, key accomplishments, and collaborations.

Computational Physics Group

Group Leader: Tarabay Antoun

The Computational Physics Group's expertise is in modeling, mechanical engineering, physics, chemical engineering, applied mechanics, computational physics, applied physics, applied mathematics, and applied science. Future directions are combining explosion modeling with atmospheric transport. Staff is currently working on LDRD, BES, DNT, NAI, Test Readiness, ASC (Containment), A Div, B Div, UGAPS, DTRA (ACTD), and DARPA.

The Computational Physics Group of the Energy and Environment Directorate focuses much of its effort on improving current understanding of the response of geologic media to strong shock waves, and on the interaction of those waves with underground structures. In recent years, the group has also established a high fidelity computational capability for simulating the interaction of energy emanating from nuclear detonations with chemical and biological agents stored in bunkers.

Two codes— LDEC and GEODYN – are developed and maintained in the group to perform most simulation. GEODYN is a Eulerian Godunov code with adaptive mesh refinement capabilities. Among its many features, GEODYN includes high-order interface reconstruction algorithms, and advanced constitutive models that incorporate salient features of the dynamic response of geologic media. LDEC is a 3D code for simulating the stability of openings in fractured rock masses. LDEC represents the rock mass using a large number of polyhedral blocks that interact at their points of contact according to experimentally validated contact force laws. Both codes are three-dimensional and massively parallel, and they are both routinely used on many of LLNL's largest high performance computing platforms.

Members of the Computational Physics Group are among LLNL's most knowledgeable and most experienced users of the laboratory's high performance computing platforms. During the MCR¹ *science runs*, members of the group used the GEODYN code to perform a 3D simulation of the Baneberry underground nuclear test. The computational model used included about 50 million zones and the simulation required approximately 40000 CPU hours to complete, thus making it the largest simulation of its kind. The simulation helped establish a new capability to perform underground test containment simulations in 3D thus making it possible to accurately represent complex geologic features in the simulation. This simulation was featured as an ASCI Highlight.

¹ MCR is a 2300 CPU computing platform. When the simulation was performed, MCR was one of the five largest computers in the world.

As part of *science runs* on THUNDER², members of the Computational Physics Group used LDEC to perform simulations of unprecedented scale to evaluate the response of a deeply buried tunnel complex in a jointed geologic medium to explosive loading. The simulation, which included about 100 million computational elements and required about 500000 CPU hours to complete, represented a fundamental change in the way simulations of large-scale underground structures are performed. By directly simulating the discrete, blocky nature of rock masses, LDEC takes a fundamental approach to simulating the behavior of these systems while limiting the number of empirically derived model features. This approach is analogous to the application of molecular dynamics where complicated results observed in simulations are emergent consequences of a large system with relatively simple, fundamental laws at work at the small scale.

The Computational Physics Group is currently made up of one postdoctoral fellow, four retirees (three of the retirees are laboratory associates and one is a contributing guest), and eight staff members with Ph.D. degrees in applied mathematics, engineering mechanics, high energy density physics, and various engineering disciplines. An additional postdoctoral fellow is expected to join the staff this summer

DOE and DoD sources fund the majority of the research performed in the group. Programs related to Defeat of Hard and Deeply Buried Targets (HDBT) account for about a third of the group's budget. Containment science and test readiness activities account for about a quarter of the budget, followed by programs for studying agent defeat, dynamic fracture, penetration, hypervelocity impact phenomena, and domestic nuclear event attribution.

Applied Geophysics & Geospatial Analysis Group

Group Leader: Phil Harben

The Applied Geophysics and Geospatial Analysis Group's expertise is in applied geophysics, seismology, GIS, earthquake hazards, geomechanics, geophysical imaging, InSAR, satellite imagery, geophysical/geological modeling, fluid mechanics, and geophysical field operations. Staff is currently working on: GNEM Program support, Geothermal Program, intelligence support (InSAR, geophysical modeling), Stockpile Stewardship support (hydrodynamic modeling), UGAPS support (geomechanics), and California Energy Commission (GIS, seismology). Future directions include: 1) integrated geospatial analysis capability combining GIS, imagery, InSAR, and geological modeling expertise applied to E&ED, National Security, and Homeland security problems, 2) develop a core oil shale technology base that provides the modeling capability and laboratory rock property measurement expertise to analyze and optimize in-situ heating processes for reservoir exploitation, and 3) build a generalized sensor and monitoring field capability that supports many communication methods and acquisition platforms.

² THUNDER is a 4000 CPU computing platform. When the simulation was performed, it was the second largest computer in the world.

Atmospheric Flow, Transport & Hazard Assessment Group

Group Leader: John Nasstrom

There are eighteen scientists and engineers in the Atmospheric, Flow, Transport and Hazard Assessment group. Eight members of the group specialize in managing and supporting major development and operational application projects within the National Atmospheric Release Advisory Center (NARAC) at LLNL. Ten members of the group conduct research and development of atmospheric flow, transport, turbulence and diffusion models for distance scales ranging from building scale to regional scale, with a focus on current and future NARAC capabilities. The group's expertise includes (1) operational meteorology and forecasting, (2) building-scale, boundary-layer, urban-scale, cloud-scale and regional-scale atmospheric flow, transport and diffusion modeling, (3) fast-response analytical-empirical atmospheric plume modeling, (4) particle deposition and resuspension, (5) precipitation scavenging, (6) nuclear fallout modeling, (7) airborne tracer and flow experiments, (8) inverse modeling for source characterization and event reconstruction, (9) ensemble and probabilistic flow and transport prediction, and (10) uncertainty estimation.

The group's staff primarily supports the NARAC-IMAAC program (see separate program description). For this program, the staff is currently working on emergency response modeling systems for DHS under the recently established Interagency Modeling and Atmospheric Assessment Center (IMAAC), and for DOE under the long-running National Atmospheric Release Advisory Center (NARAC) program. For DHS and LDRD projects, the group is actively working on urban atmosphere flow and diffusion modeling, tracer field experiments for model validation, and event-reconstruction/sensor-data-driven modeling. The staff also supports several national and homeland security projects in the LLNL NAI directorate, providing airborne hazard modeling expertise. The NARAC emergency operations center and computer center are major resources supported and utilized by the group.

The members of the group and their highest degrees are as follows:

Fernando Aluzzi, M.S., Meteorology
Ron Baskett, M.S., Atmospheric Science — Deputy Group Leader
Michael Bradley, Ph.D., Atmospheric Science
Stevens Chan, Ph.D., Engineering
Steve Chin, Ph.D., Atmospheric Science
Luca Delle Monache, Ph.D., Atmospheric Science (Post-doc)
Michael Dillon, Ph.D., Physical Chemistry
Connee Foster, M.S., Atmospheric Science
Kevin Foster, M.S., Atmospheric Science
Peter Goldstein, Ph.D., Physics
Branko Kosovic, Ph.D., Aerospace Engineering
Marty Leach, Ph.D., Meteorology

John Leone, Ph.D., Meteorology
Gwen Loosmore, Ph.D., Civil and Environmental Engineering — Deputy Group Leader
Julie Lundquist, Ph.D., Astrophysical, Planetary & Atmospheric Science
Jeff Mirocha, Ph.D., Atmospheric Science (Post-doc)
Brenda Pobanz, M.S., Atmospheric Science
Phil Vogt, M.S., Meteorology

Major computer codes developed and utilized by the group include the following:

- ADAPT meteorological data assimilation model,
- LODI Lagrangian particle atmospheric dispersion model,
- COAMPS regional weather forecast model (in a collaboration with the Naval Research Laboratory), and
- FEM3MP and AUDIM building- and urban-scale computational fluid dynamics models.

The success of our group and the programs we support depends on multi-disciplinary collaboration to develop advanced real-time modeling systems that span from sources to effects to emergency response information. Major, active collaborations are maintained with several LLNL Directorates, including Computations, Engineering, NAI, DNT and SEP. The following is a list of external collaborating organizations, collaborator names, and areas of research:

- UC Berkeley: Fotini Chow, urban atmospheric turbulence, event reconstruction
- NCAR: Tom Warner, operational forecasting incorporating nowcasting and variational data assimilation
- NOAA/ Field Research Division: Kirk Clawson, field experiments
- NOAA Aeronomy Lab/CIRES: Wayne Angevine, boundary-layer height prediction and quantification
- University of Colorado/CIRES: Jeff Weil, turbulence and diffusion model parameterizations
- NOAA Hazardous Material Response and Assessment Division: Mark Miller, chemical hazard databases and models (CAMEO/ALOHA system)
- NRC: Stephen Mcguire, nuclear power plant accident source characteristics (RASCAL code)
- ESRI, Inc. and DOE Remote Sensing Laboratory RSL, interfaces between modeling systems and GIS software
- LBNL: Ashok Gadgil and Rich Sextro, Indoor exposures
- UK Defence Science and Technology Laboratory (dstl): Ian Griffiths, Empirical urban model
- NRL: Julie Pullen and Teddy Holt, Mesoscale modeling and COAMPS
- PNNL: Jerry Allwine, Urban Dispersion Program
- LANL: Michael Brown, Urban Dispersion Program
- LANL/ORNL: Geospatial population density databases
- ORNL: Keith Eckerman, Acute and chronic radioactive dose and risk models

- SNL: John Fulton, casualty/fatality estimates and prompt effects from nuclear explosions
- SNL: Fred Harper and John Brockmann, Radiological, chemical and biological source characteristics
- U.S. Army ECBC: Ray Jablonski, Dose-response relationships and toxic load models for chem./bio.agents

Energy Conversion and Storage Group

Group Leader: Sal Aceves

The group's vision is to assure that the nation's future energy demands can be met in an environmentally responsible manner. Current work addresses this important problem through multiple parallel efforts.

- Developing technologies that will enable us to stabilize the global climate while providing the energy demands of modern living. This is accomplished through development of hydrogen energy technologies that will enable a viable hydrogen economy. Other carbonless energy carriers are also being investigated.
- Increasing the efficiency of existing energy technologies while minimizing their environmental impact. This is done by optimizing energy systems and improving conversion efficiencies in engines and fuel cells.
- Reducing environmental impact of existing energy technologies. This is addressed by improved combustion of fuels at more uniform temperatures to reduce NO_x, and developing sensors for internal combustion engines.
- Partnering with industry to commercialize our technology. We have licensed our Inductrack magnetic levitation system for high-speed trains. We have collaborations with Ford, BMW, General Atomics, Caterpillar, International and Cummins.

The Group's expertise is in mechanical engineering, physics, analytical chemistry, hydrogen storage and usage, combustion engineering and modeling, and energy flow modeling. Staff is currently working on hydrogen, combustion, sensors, energy modeling, and DNT. Future is in development of technologies for reducing CO₂ emissions through energy efficiency and carbonless energy carriers.

The group has 10 members. Four of the group members (Aceves, Edman, Flowers, and Killingsworth) are mainly dedicated to detailed modeling of advanced combustion technologies for internal combustion engines. This includes chemical kinetics of reacting mixtures, modeling of fuel injection processes, and combustion control. A group member (Berry) is dedicated to hydrogen technologies and energy modeling. Bob Glass works on sensors for emissions controls and as a program manager for the California Energy Commission. Espinosa-Loza works on analysis and demonstration of innovative hydrogen storage technologies. Smith works on Defense Technologies, conducting modeling of weapon systems. Post is a retiree who works on magnetically levitated trains, plasma systems and energy storage in flywheels. Ross is an engineering associate who designs and conducts experiments for hydrogen storage and internal combustion engines.

The group has an internal combustion engine test facility located in B435 where the high efficiency and low emissions of HCCI (homogeneous charge compression ignition) technology are being demonstrated. Another facility is the cryotank laboratory, where

hydrogen storage vessels are being built and tested. The group also owns a hydrogen trailer in the trailer yard to conduct hydrogen refueling experiments. Much of the hydrogen tests are conducted at the high-pressure laboratory (B235).

We are in the process of receiving a hydrogen-fueled Toyota Prius vehicle, which will be used as a moving laboratory to conduct hydrogen storage technology experiments. We have developed advanced analysis tools that have made us world leaders on HCCI combustion. These codes are used in our collaborations with Cummins as well as International engines.

The group has been able to maintain and grow its funding through a very difficult budget year. Group members have been able to establish solid relationships with DOE program managers who believe that they get good value for their investment.

Our external prestige has also increased. Group members are frequently invited to write papers and deliver seminars in prestigious venues. Several patents have recently been written.

Nuclear & Risk Science Group

Group Leader: Bob Budnitz

The Group's expertise is in various engineering disciplines (nuclear, mechanical, electronic, civil, and chemical engineering) as well as in environmental science, risk analysis, quality assurance, and program management. Staff members are currently working on a wide variety of projects, including the Yucca Mountain project, nuclear-reactor advanced development, safeguards technology work, work on environmental impacts of existing LLNL operations at the Nevada Test Site, energy policy studies, work in Russia to monitor the Russian uranium-downblending program, nuclear fuel-cycle advanced system design, non-proliferation and nuclear-security policy development, nuclear power-plant safety emphasizing PRA methods and seismic safety, and NRC regulatory analysis of new reactor sites.

The Group consists entirely of mature professionals, all with 25 or more years of experience. Also, essentially every member of the Group works on smaller projects in a self-directed mode, rather than in larger projects under close supervision. The Group members typically generate their own ideas for new projects. They usually deal directly with their DOE and NRC sponsors, and usually formulate next year's work through such interactions. The vast majority of the Group's projects are of this kind, although a few Group members work on projects that are much larger, of longer duration, and have a project leader responsible for all of the interactions with the sponsor.

Some Group members support work in other LLNL Directorates, principally in the NAI, CMS, and Engineering Directorates. However, most of the Group's project work is in our own E&E Directorate. None of the Group members performs experimental work.

One major future direction is expected to be supporting DOE's new "Global Nuclear Energy Partnership" (GNEP) that plans to develop advanced nuclear reactor and fuel-cycle technologies. Other new work is likely to involve DOE and NRC programs that will support an expected domestic resurgence of nuclear power. If the GNEP initiative becomes a major new program in DOE, the expectation is that this Group will need to expand both in numbers and in expertise. The new expertise will probably need to be in nuclear fuel-cycle technology, systems analysis, and radioactive-waste-disposition technologies.

Key recent accomplishments exist in each of these areas. One major accomplishment is that several of the Group's members provided important technical support to DOE as the Department spent the last several months developing what has become the new GNEP initiative.

Climate/Carbon Science Group

Group Leader: Dave Bader

The Climate/Carbon Group's expertise is in: global and regional climate model analysis with an emphasis on comparison of models to data, global climate model parameterization development, synoptic to global scale numerical weather prediction, coupled carbon cycle- climate model development and application, atmospheric radiative transfer, atmospheric chemistry and aerosol model development and application, and modeling of climate change impacts. Staff is currently working on the Climate Change Prediction Program (PCMDI, SciDAC), Atmospheric Radiation Measurement Program (ARM Science Team, ARM Infrastructure) and Atmospheric Science Program (ASP) for DOE Office of Science. Also, NASA's Modeling Analysis and Prediction and regional and high-resolution global climate modeling and land surface change for LDRD and California Energy Commission.

Geochemistry Group

Group Leader: Carol Bruton

The Geochemistry Group specializes in studies of complex chemical, physical and biological interactions in natural and engineered systems. We integrate laboratory experiments, computer simulations and field studies to credibly forecast outcomes at multiple spatial and temporal scales, provide data to quantify uncertainty, and address problems of local to national significance. We maintain a spectrum of geochemical expertise and capabilities to support and develop LLNL programs. Areas of expertise of group members include: thermodynamics and kinetics, geology, geochemistry, aqueous, surface, physical, analytical and radionuclide chemistry, water-rock-material interactions, soil science, and technical laboratory and field support. The group is composed of fifteen

people. Eleven group members possess Ph.D.s and three have M.S. degrees. We have one post-doc and a post-college appointment. Carol Bruton and Bill Bourcier serve as group leader and deputy group leader, respectively.

The Geochemistry Group provides support to a number of E&ED and LLNL programs. In the Yucca Mountain Project (Nuclear Systems Science and Engineering Program), group members have held management positions and conducted research in brine chemistry that can potentially corrode metal waste containers. Group members also provide environmental support to national security programs such as DNT through the Underground Test Area Project (UGTA) at the Nevada Test Site. In UGTA, we apply our expertise in contaminant fate and transport to conduct computer modeling and laboratory experiments of glass dissolution and radionuclide sorption. We also collaborate with the Flow and Transport Group to conduct reactive transport modeling of radionuclide transport in the subsurface for UGTA. Our chemical expertise and experience in conducting field campaigns are utilized in CAMS and the Marshall Islands program.

Our support of the Earth Systems Science and Engineering Program extends to the Carbon Management, Water and Environment, and Energy Systems subprograms. We are nationally recognized for our reactive transport modeling of fluid-rock interactions accompanying CO₂ sequestration and enhanced oil recovery, and we are expanding these models to provide for injection of gas mixtures and the integrated chemical-mechanical effects of injection (Carbon Management). We have a new program in water treatment technology, begun through an LDRD investment, which is attracting Work-for-Others funding and producing novel technologies for desalination and selective extraction. We also work within the Safety and Environmental Protection Directorate to develop new funding opportunities for water research at LLNL (Water and Environment). Our work in geothermal energy extends from California Energy Commission-funded studies of by-product recovery from geothermal brines, to management responsibility for the Geothermal Program at LLNL (Energy Systems).

LDRD and Basic Energy Sciences support multiple fundamental research projects within the group. Current projects include the impact of chemistry on fracture mechanics, experimental, modeling and field studies of the performance of geologic CO₂ storage sites, and novel means of stripping CO₂ from gas mixtures.

The Geochemistry Group maintains a variety of laboratories and analytical facilities. B243 contains most of the high-pressure and specialized chemical reactor systems for studying geothermal and accelerated natural processes. B281 contains extensive laboratories for conducting experiments on natural systems and analyzing organics, inorganics, and biochemical systems and is capable of handling low-level radioactive samples. Both facilities contain general chemical laboratories.

We use a wide variety of highly specialized chemical reactor systems, both closed and flowing, that span temperature and pressure space from sub-ambient to 500°C and 2 kb. Most of these are constructed of noble metal or otherwise chemically inert materials. They are used to measure basic thermodynamic and kinetic properties of minerals, as

well as to conduct model validation experiments and chemical engineering experiments to support lab programs. Analytical equipment associated with these studies include a variety of highly sensitive surface analytical techniques for characterization of experimental samples, ranging from the atomic scale (conventional and hydrothermal atomic force microscopy, scanning interferometers, etc.) to macroscale (BET surface analyzers, x-ray diffraction, gas chromatographs, GC-mass spectrometers, dynamic light scattering instrument, etc.) to solution chemistry analytical devices (inductively coupled plasma emission spectroscopy, graphite furnace atomic absorption spectroscopy, ion chromatography, colorimeters, etc.).

Our capability for organics analysis in B281 includes gas and liquid chromatography, mass spectrometry, ultraviolet spectroscopy, and infrared spectroscopy. A general-use inorganic solution chemistry measurement capability is also maintained in B281, including inductively coupled plasma emission spectroscopy, graphite furnace atomic absorption spectroscopy, ion chromatography and colorimeters. To support atmospheric and meteorological field tests, we also maintain and operate much of the measurement capability for tracer tests, such as field sampling, analytical and meteorological equipment.

We have recently added a water treatment laboratory to test and develop new technologies for desalination and selective extractions. The laboratory contains a membrane testing unit, commercial electrodialysis unit, an LLNL-patented carbon aerogel capacitive deionization unit (CDI), and equipment for testing a new technology for desalination, the ion pump, being developed at LLNL.

Geochemistry Group members collaborate with a variety of external institutions, such as the California Institute of Technology, University of Southern California, U.C. Santa Cruz, U.C. Los Angeles, Wright State University and Texas Christian University. We also collaborate with local water utilities and agencies, and our industrial partners. Notable achievements during the past year include participation of a group member as Theme Leader for Phase-II geochemical modeling and monitoring activities for the international Weyburn CO₂-flood enhanced oil recovery and sequestration project (Saskatchewan, Canada). Another group member serves in an IJE position with the Geothermal Program of the California Energy Commission, responsible for project management, solicitations, and enhancing the Commission's knowledge base in direct-use geothermal applications and research needs. We have two patents pending and have filed four records of invention for novel water treatment technologies.

CAMS Group

Group Leader: John Knezovich

See CAMS Program Section

Experimental Geophysics Group

Group Leader: Rick Ryerson

The Experimental Geophysics Group's expertise is in: rock and mineral physics (high P-T measurements, phase equilibria and EOS, electrical conductivity, deformation, elastic phonon dispersion, wave propagation, reactive chemical transport, and spectroscopy). The group currently includes 11 Ph.D. staff scientists, 3 technicians and 3 postdoctoral associates. Current work includes: fluid-flow through fractures, electrical conductivity of partially saturated lithologies and mantle rheology for BES, Mission to Really Early Earth and The Chemistry of Core Formation through the IGPP-LDRD portfolio., equation-of-state of "specialty metals" and powders, Pu metrology, phonon spectroscopy of "specialty metals" for DNT, two LDRDs: Kinetics/Ultrasonics of Phase Transitions with DNT, and Salton Sea Rock-Fluid Interactions with the Geothermal Program, Las Vegas Basin Strong Motion project for YMP, and several WFO projects. Future directions include: increased interactions with DNT, GNEM, BES High-Pressure Research, radiation detection (NAI), materials characterization DNT, CO₂ Sequestration, Oil Shale, CAMS connections, YMP strong motion and clathrate properties w/ seafloor electromagnetic methods consortium.

Environmental Science Group

Group Leader: Gayle Pawloski

The Environmental Sciences Group is very diverse. It represents competencies in biology, analytical and organic chemistry, environmental science, geology, meteorology, toxicology, and health effects. People in the group have a range of degrees, including Ph.D., MS, BS, AA, and no degree.

The group consists of: Ken Bogen, Jim Brunk, Cindy Conrado, Jeff Daniels, Frank Gouveia, Sheilah Hendrickson, Jim S. Johnson, Garrett Keating, Steve Kehl, Jim Kercher, Sue Martin, Roald Leif, Ariel Rivers, Marshall Stuart, Bill Robison.

We support field deployments collecting air, biota, soil and water sampling. We perform laboratory analyses for characterization, signature and threshold determinations, and model input. We perform health and risk assessments including dose response, risk assessment, exposure analysis, and applied statistical analysis. We also develop methods that improve field sampling, laboratory analysis, and assessments. The strength we want to build on is integrated environmental assessments, where we development methods to collect data, provide laboratory analyses, and perform assessments to address specific scientific and programmatic issues.

People in this group support a large number of programs. Only about one third of the group members work for a single program. Many members support at least two programs and sometimes up to four. Group funding comes from both inside (35%) and outside

(64%) the Directorate. Within the Directorate we support field deployments, laboratory analysis, and environmental and health assessments for the Marshall Island (MI) Program; we perform laboratory analyses for Yucca Mountain Program (YMP); we provide unique meteorological data analysis for the Knowles Atomic Power Laboratory (KAPL) to support their annual environmental assessment; we provide particle analysis in an aerosol chamber supporting an EPD LDRD project; and we provide data compilation, analysis, and health assessments investigating food mutagens and prostate cancer of African American on a 5-year National Institute of Health grant. For the Defense and Nuclear Technologies Directorate (DNT) we provide management to the earth science applications of the Underground Test Area (UGTA) Program investigating radionuclide migration at the Nevada Test Site; we support the Stockpile Stewardship Readiness Program through the Containment and Nuclear Chemistry programs; we perform B-Division physics analysis and code support on deflagration of He before detonation. For the Safety and Environmental Protection Directorate (SEP) we provide laboratory analysis and methods development to the Groundwater Ambient Monitoring and Assessment (GAMA) Project; regulatory water sampling; and analysis and project support for environmental re-permitting. We also support the Nonproliferation, Arms Control, and International Security Directorate (NAI) Bioaerosol Mass Spectrometry (BAMS) Project with methods development for detection and identification of low concentration spores in short time periods; a skin decontamination project; system studies of health effects; field deployment and laboratory analyses for the urban dispersion projects; and radionuclide material protection, control, and accounting expertise between the US and the Former Soviet Union. We manage a gamma spectroscopy laboratory for the Chemistry and Material Sciences Directorate (CMS), analyzing environmental isotopes and various radionuclides for SEP, the Forensic Science Center, International Atomic Energy Agency (IAEA), Domestic Nuclear Event Attribution (DNEA), Mare Island Project, and other projects and agencies.

Members of our group are responsible for maintaining several laboratories in buildings 281, 378 and 379. We measure organics in water and air, various biologics in air and on skin, and low-level radiochemicals in soil, food, and ecological samples. We are responsible for large historical archives of data for the Marshall Islands and Containment programs. Matrixed members of our group manage bioaerosol and nuclear chemistry laboratories in CMS.

Seismology Group

Group Leader: Arthur Rodgers

The Seismology Group is composed of 14 Ph.D. researchers (200 series) and one Scientific Associate (300 series). Expertise in the group is strongly focused on nuclear explosion monitoring, but also includes signal processing, seismic event location, earthquake-explosion discrimination, estimation of seismic velocity structure, computational seismology, and field seismology.

The Seismology Group performs research to support national security and earth science programs. The primary sponsor of work in the group is the Ground-Based Nuclear Explosion Monitoring (GNEM) Program, funded by NNSA/NA-22. Smaller programs in the group support theoretical and experimental geophysical studies and regional cooperation in seismology.

The GNEM Program supports significant computational and archival systems used by all Seismology Group members. These include a network of SUN, Apple and PC workstations, a 54 CPU LINUX cluster and RAID system. An Oracle database with millions of event-segmented seismic waveforms is used extensively by the group. Data are accessible through a set of GNEM-developed tools that enable interactive measurement and analysis for research products. A new elastic finite difference code is being developed for parallel computation of seismograms in three-dimensionally heterogeneous earth models. Field experiments are supported by a geophysical observatory capability including numerous systems for remote autonomous deployment.

The group collaborates extensively with seismologists in the U.S. and abroad and has many strong collaborations with institutions in the Europe, Middle East and South Asia. There are strong ongoing collaborations with seismologists at UC Berkeley and UC Santa Cruz. The group actively travels both domestically and abroad for programmatic meetings and conferences. These activities involve approval processes for hosting foreign nationals at the Lab (including LLNL employees) as well as foreign travel, including sensitive countries.

Flow and Transport Group

Group Leader: Andy Tompson

The group's expertise is in hydrogeology, hydrology, thermal hydrology, reactive transport and geochemistry, computational science, geology, geophysics, and geostatistics, physics of multiphase flow in porous media, fluid and rock mechanics, petroleum and mechanical engineering, isotope chemistry and risk and consequence analysis. Staff is currently working on YMP, UGTA for DNT, regional security projects for NAI, information security project (PAT), ERD Remediation projects and GAMA project for SSEP, Salton Sea project, High Explosives Modeling Project for DNT, Heavy Vehicle Aero Project, groundwater, land surface and regional climate model and clay fracture project (LDRD), NARAC, FSC for CMS, Toxic Industrial Chemicals project for NAI/DHS, Geologic Carbon Sequestration and Dominguez Channel project. Future research interests include: "... address coupled and more diverse flow, mass transport, and ecological problems intersecting atmospheric, land surface, estuarine, and subsurface environments. Areas and issues under consideration include water resource management, regional climate, fate and transport (e.g., pollutants, isotopes, pathogens, NBC agents, carbon, etc.), and collaborations across a greater spectrum of institutional, academic, and government/agency sponsors.

Energy and Environment Programs

NARAC/IMAAC Program

Program Leader: Gayle Sugiyama

Hazardous airborne releases are one of the most rapid and effective means to impact large populations. The mission of the NARAC/IMAAC Program is to provide critical information during such events, in order to save lives and mitigate consequences as part of an integrated national preparedness and response strategy. The program spans research to operations and is coupled to the broader suite of LLNL's end-to-end technologies, expertise base, and operational capabilities for countering and responding to WMD (weapons of mass destruction) and terrorist threats.

The NARAC/IMAAC Program has achieved significant growth in recent years. The selection of the National Atmospheric Release Advisory Center (NARAC) as the interim provider of capabilities for the new Department of Homeland Security's Interagency Modeling and Atmospheric Assessment Center (IMAAC) in April 2004 was a key milestone. Since that time, we have successfully provided IMAAC operational services and are collaborating with the IMAAC agencies (DHS, DoD, DOE, EPA, NOAA, NASA, and NRC, with the planned addition of HHS and DOT) to develop a coordinated national response to hazardous atmospheric events. In addition, our primary DOE sponsor has identified NARAC as the "reachback" modeling asset for the Nuclear Incident Response Teams and required connectivity to NARAC by all DOE facilities with the potential for off-site releases.

A robust science and technology development portfolio is critical to the long-range success of the NARAC/IMAAC Program. We are conducting cutting-edge research in strategically important areas, including urban (outdoor and indoor) modeling, event reconstruction (data-driven simulation for characterizing unknown source terms), and key transport and transformation processes. A systems modernization effort is underway to address multiple simultaneous events, a potentially massive expansion in usage, better/faster/more cost effective operations, and the integration of advanced simulation capabilities.

National Security Preparedness & Response: Operational Status

The center supports an ever expanding customer base, which currently consists of more than 300 collaborating local, state, and federal organizations and emergency operations centers (Table 1) and over 1700 on-line users. Over the last year, we responded to:

- More than 5000 automated tests and drills by end-users
- Over 100 local, state, regional, and national exercises, involving extensive LLNL staff involvement with planning and execution
- 2-4 major national exercises (National Exercise Program)

- ~20 real-world events, including NSSEs (National Security Special Events), alerts, and emergencies (see Table 2)
- Technical support requests for threat assessments (e.g., DHS/HHS Material Threat Assessments and Systems Studies) and infrastructure/facility protection risk analyses (e.g., DHS Infrastructure Protection and U.S. Secret Service vulnerability studies for toxic industrial chemical facilities or transportation modes)

Some recent examples of NARAC/IMAAC supported events include:

- Top Officials 3 (TOPOFF3) exercise - a biannual cycle of preparation and training, culminating in a full-scale exercise based on a coordinated terrorist incident, involving weapons of mass destruction scenarios (2005 April 6-9)
- Pinnacle exercise (2005 July)
- BioWatch detection events (2005 October-November)
- Pluto New Horizons satellite launch (2006 January)
- Real-world chemical accidents, e.g., 2005 February 25 New York City warehouse fire and 2005 August 30 Cincinnati tank car spill (see Table 2)
- State-of-the-Union address (2006 January 31 NSSE)

NARAC/IMAAC Strategy and Progress

The program's strategic objectives are focused on the continued maintenance and expansion of our mission space, operational capabilities, stakeholder base, and science and technology portfolio. Over the past several years, we have successfully transformed NARAC from a specialized center, with a relatively limited role in DOE facility protection and nuclear incident response, to become the national center-of-excellence for real-time assessments of the potential impacts of airborne hazardous materials releases. Two key next steps in our strategy are discussed below.

Strategic Planning

A "Blue Sky" workshop was held in July 2005 to solicit input on whether the center might be asked to respond to disasters that are far beyond our current capabilities and/or sponsor expectations. The workshop brought together a variety of LLNL experts (external to the program), who are familiar with possible disasters, terrorist activities, and accidents that could generate airborne hazards. Discussions were conducted at the SRD classification level. The workshop identified event management as the most critical issue deserving attention, specifically the need to address:

- Multiple (simultaneous or sequential) events
- New or unexpected threats (responding to the unknown)

Workshop participants also prioritized the importance of:

- Analysis tools that provide information on the location, timing, and methods used in chemical or biological attacks, with the goal of utilizing this knowledge to mitigate or even forestall sequential "reload" attacks

- Continuing efforts to provide user-friendly “actionable information” for decision makers and responders
- Development efforts focused on model improvement, validation, and uncertainty estimation

IMAAC: Site Selection Process

The IMAAC continues to be a focal point of our strategic plan. Under the National Response Plan, the IMAAC “provides a single point for the coordination and dissemination of Federal dispersion modeling and hazard prediction products that represent the Federal position during an Incident of National Significance”. The Homeland Security Council’s designation of NARAC as the interim IMAAC validated the program’s successful development strategy. The center was also recognized by its inclusion on the short list of LLNL facilities visited by DHS Secretary Chertoff on July 27, 2005.

The selection process for the permanent site of the IMAAC is currently underway. On February 1, 2006, LLNL hosted a visit by a site survey team, including three members of the IMAAC Scientific Advisory Group (SAG), who will be recommending possible options to the Interagency Working Group (IWG) and Senior Management Council (SMC). The program presentations and center capabilities received uniformly positive feedback from the visitors, as well as NAI AD Ray Juzaitis. We have been requested to provide a similar detailed review to Kirk Evans (SMC Chair, Director of the Office of Program, Plans, and Requirements, DHS Science and Technology Directorate). The program also has the endorsement of DOE/NNSA Deputy Under-Secretary for Counterterrorism Steve Aoki (SMC DOE representative) to site the IMAAC at LLNL.

As part of the site selection process, we proposed a concept for an interagency IMAAC, based on a core LLNL center networked to affiliated IMAAC organizations. In this concept, we would:

- Provide access to LLNL’s full suite of advisory services proven over 27 years of operations (24x7 expert staff, comprehensive suite of models, real-time operational system, supporting infrastructure, remote-access systems, and coupled R&D program)
- Leverage multi-sponsor investment to provide enhanced infrastructure, increased capacity, and surge capacity (personnel, hardware, and tools)
- Extend and formalize LLNL’s collaborative operational relationships and foster interagency coordination as part of the national preparedness and response strategy
- Expand the IMAAC user base, via interagency quotas, user vetting, and training
- Provide cost-sustainable state and local support by drawing on existing IMAAC agency regional emergency response assets and lessons learned from the Local Integration of NARAC with Cities (LINC) program
- Build up an extended network of interagency subject matter experts, integrated with LLNL’s existing national laboratory and agency contacts
- Support an interagency VV&A (verification, validation and accreditation) process

- Integrate additional IMAAC accredited modeling tools
- Expand LLNL's portfolio of collaborative R&D projects
- Create an IMAAC User Group and an IMAAC Technical Requirements Group
- Host an IMAAC Visiting Scientist Program
- Leverage other LLNL site resources including security infrastructure and computational resources

Many of the needs identified by the “Blue Sky” workshop are reflected in the IMAAC concept. Existing and planned efforts to address these requirements include upgrading our surge capacity, network of subject matter experts, and scientific and operational capabilities, as discussed in the following sections.

Event Management: Multiple Event Support

The center regularly supports multiple concurrent events (exercises, drills, real-world responses). The number of large-scale events (or Incidents of National Significance) that can be handled is a strong function of the complexity of the analysis required and is primarily limited by the availability of expert staff. For example, responding to covert large-scale biological releases or new threat agents will be extremely manpower intensive and harder to sustain for extended periods.

Personnel Surge Capacity. Center staffing and infrastructure are maintained with the goal of supporting two simultaneous major incidents 24x7 for a two-week period. Beyond that time frame, we depend upon cross-trained software and model development staff from our program, provided with supplemental just in time training as needed. We are currently addressing the need for additional personnel surge capacity via a combination of the following activities:

- A limited expansion of our core multidisciplinary staff (over the past year, we have hired two new operational scientists, a health physicist, a model developer and two postdoctoral scientists for a total of 50 program personnel)
- Training and integration of additional LLNL subject matter experts and users
- Development of access to additional trained manpower from our operational collaborators and supported customers (Table 1)

Under the IMAAC umbrella, our surge capacity could be strengthened by drawing on hundreds of new users from federal emergency response assets, as well as state and local stakeholders.

System Surge Capacity. The current third-generation NARAC software system became operational in 2000. It is a fully automated client-server system, which can handle multiple simultaneous users and events. Internet technology (NARAC iClient and Web) connects remote users to the center. Multiple systems provide redundancy for fault-tolerance, backup, development, and testing. This system has supported an explosive growth in our customer base and event responses in recent years, with a minimal increase in operational staff.

A design plan has been drafted to create a next generation system designed to support 5-10 simultaneous events, 50 simultaneous simulations, and 500 simultaneous external users. We are currently taking incremental steps towards the development of this system (as supported by current funding levels) including:

- Completing the porting of the system to Linux
- Further scalability enhancements to the center's hardware and software systems
- Prototyping the use of LLNL's high-performance computing platforms to support advanced simulation tools and improve response times (Note: during a recent real-world event, we tested the ability to use computational surge capacity from LLNL's institutional supercomputing resources)
- Improvements to ease integration of additional models

Operational Response Plans. Detailed response plans exist for most types of radiological and nuclear events, under DOE, DoD, EPA, and NRC auspices. IMAAC currently is building on these plans to develop Standard Operating Protocols for chemical and biological responses as well. We need to develop additional detailed plans for supporting multiple attack scenarios that would obviously exceed our normal capacity. Such protocols would specify such items as surge capacity support contacts, processes for accessing institutional computer resources, and communications handling for dealing with multiple locales simultaneously.

Event Management: Responding to the Unknown

Normal center operations depend upon the expertise provided by our core multidisciplinary staff, which provides source-to-effects analyses. As needed, we draw upon a wider network of subject matter experts including:

- LLNL collaborators with expertise in atmospheric science, chemistry, WMD, health physics and industrial hygiene, computer science, statistics, engineering, and geographical information systems
- LLNL knowledge center experts (e.g., Biodefense Knowledge Center, CAPS/HOPS, NAP, DNT)
- National laboratory collaborators (Table 3)
- Operational response assets (Table 1)

To enhance our ability to respond to novel or unexpected threats and events, we are developing contact lists of additional experts drawn from the broader IMAAC community, as well as other federal, state, and local agencies. As this list matures, a formal connectivity plan for bringing this outside expertise to bear will be put into place.

Science Research and Development

In order to cement its leading role in airborne hazards modeling, the NARAC/IMAAC Program pursues strategic R&D thrust areas, as well as the continuous development, integration, and evaluation of new simulation tools (both in-house models and tools supplied by external collaborators).

R&D thrust area: Urban models. Due to the potential for high population and infrastructure impacts, a critical need exists for simulation capabilities that provide accurate airborne hazards predictions for urban areas. LLNL efforts to understand and model urban transport and physics include the following:

- **Urban field studies.** The Joint Urban 2003 field study in Oklahoma City was the largest and most complex urban tracer experiment performed to date. Data analysis has led to a better understanding of the turbulent kinetic energy balance in urban areas and the importance of incorporating mesoscale forcing. LLNL is currently participating in the DHS Urban Dispersion Program, which is conducting further urban field studies in New York City.
- **Urban model development.** LLNL is developing a multiscale suite of models to simulate the flow and dispersion of airborne agents within urban areas. This effort includes development of urban canopy models as well as computational fluid dynamics (CFD) models, which explicitly incorporate the effects of individual buildings. Evaluation of our CFD building-scale model against urban field study data has shown that we can successfully simulate detailed features of atmospheric transport in urban environments. Our Adaptive Urban Dispersion Integrated Model (AUDIM) is integrating new rapid geometry-to-mesh capabilities, treatment of complex building geometries, advanced numerical solvers, and state-of-the-science parallelization with our current model.
- **Urban atmospheric turbulence.** A new E&ED LDRD project is developing improved turbulence closure models from observations and simulations of the urban environment.

R&D thrust area: Data-driven simulation. In recent years, the analysis of field data to determine unknown source terms and refine predictions has become a common feature of our real-world responses. NARAC/IMAAC routinely participates in emergency response drills with organizations that collect air concentration, ground deposition, and exposure measurements. Analysis of such data can be extremely personnel intensive and relies heavily on analyst judgment. A key R&D thrust is to develop tools to assist this process.

- **Event reconstruction.** A multi-directorate LDRD project is developing a data-driven event reconstruction capability to seamlessly integrate observational data streams with predictive models in order to provide probabilistic estimates of unknown source term parameters (location, time-varying release rate). The final output of this methodology is an optimized plume prediction, including confidence levels. A robust methodology based on Bayesian inference and stochastic sampling has been coupled with a variety of predictive models to treat multiple resolutions. The approach has been successfully applied to complex and moving source scenarios; regional-scale tracer experiments using the NARAC/IMAAC operational models; and building-to-urban scale CFD scenarios.
- **Uncertainty estimation.** The atmospheric and emergency response communities have identified the need to understand and communicate model uncertainty as a high research priority. Ensembles and event reconstruction provides two starting points for this analysis, but additional R&D efforts are needed.

Collaborative integration of external simulation tools. NARAC/IMAAC's goal is to supply a complete range of validated simulation tools to model the behavior of hazardous radiological/nuclear, chemical, biological, and natural (e.g., smoke, volcanic) releases on global, regional, urban, and building scales. Simpler, fast-running deployable models are used to perform screening calculations, support fast initial response, and provide functionality that does not require connectivity to LLNL. Detailed three-dimensional dispersion models, coupled to real-time observational data and numerical weather prediction model output, are used for near-real-time response and detailed assessments. Our modeling suite contains externally developed tools, as well as in-house models, and we are currently integrating the following capabilities provided by our collaborators:

- An empirical urban dispersion model (U.K. Dstl Urban Dispersion Model)
- Residential and commercial building infiltration models to predict indoor exposures (LBNL)
- Source characterization models for radiological/nuclear, chemical and biological releases, including nuclear reactor, RDD, IND, fire, explosive, sprayers, spill, and leak source models (LLNL, NRC, EPA/NOAA, SNL)
- Explosive and prompt effects models (SNL)
- Dose response models (ORNL, DOE/EPA/AIHA, DOD ECBC/USAMRIID)
- Supporting databases needed to generate geographical displays of hazard areas, affected populations, health effects, and protective action guidelines

Other Collaborative R&D. NARAC is engaged in a wide range of other collaborative efforts, including the following projects:

- Integration of mapping systems for field measurements, modeling results, and dose assessment to support DOE nuclear incident response capabilities, with Sandia and RSL (DOE funding)
- Development of an advanced nuclear fallout model that includes specific isotopes, respirable-size particles, underground detonations, three-dimensional and time-varying weather (w/LLNL DNT Directorate)
- Standardization with EPA/NOAA's CAMEO/ALOHA toxic chemical databases and atmospheric dispersion models (NOAA Hazardous Materials Response Division)
- High altitude dispersion for missile intercept (DoD funding, w/LLNL NAI Directorate)
- Incorporation of chemical reactions (E&ED LDRD w/Climate / Carbon Group)

On-going model and system evaluation. Evaluation and testing of the center's systems and models is a continuous priority. Model evaluation includes the use of analytic solutions (known, exact mathematical solutions to the model equations) to verify that the numerical methods used are sufficiently accurate. Comparisons against tracer field experiment data are used to test and evaluate models for a range of real-world terrain and meteorological conditions. After-action reviews following actual atmospheric release events evaluate model usability, efficiency, and reliability of models for real-world operations. Our software systems comply with DOE and LLNL SQA and C&A requirements.

NARAC/IMAAC Program Sponsors

DOE and DHS provide core funding for the NARAC operational center, supplemented by DoD and internal LLNL funding. The DOE/NNSA Emergency Operations (NA-40) Atmospheric Release Advisory Capability (ARAC) Program provides the primary base operational funding for NARAC. The DoD/DOE Naval Reactor Program uses NARAC to provide emergency response for its sites. A growing effort is DOE/NNSA's (NA-23) International Emergency Management and Cooperation (IEMC) Program, which works to strengthen worldwide emergency preparedness and to develop capabilities to respond to international nuclear accidents.

The IMAAC is funded via the DHS Science & Technology (S&T) Directorate. Additional funding is obtained from the LLNL Nonproliferation, Arms Control and International Security (NAI) Directorate / Homeland Security Office for a variety of national security applications projects.

LLNL's research and development efforts are currently supported by the DHS S&T Directorate (urban and chemical/biological agent capabilities); the DOE Technology Integration Program (radiological and nuclear capabilities); and competitive internal LLNL research funding (LDRD projects for cutting-edge capabilities such as event reconstruction). A major challenge for the program is to maintain and stabilize base R&D funding.

NARAC/IMAAC Program Organization

A new program management structure has been put in place recently, consisting of:

- Gayle Sugiyama - Program Leader
- Associate Program Leaders
 - John Nasstrom - Operations Center
 - Roger Aines - Science & Technology
- Team Leaders
 - Ron Baskett – Operational Response and Outreach
 - Shawn Larsen – Systems Development
 - Gwen Loosmore – Model Integration
 - Branko Kosovic – R&D
 - Brenda Pobanz – Operational Integration
 - Bill Eme – Customer Interface Software

Associate Program Leaders provide oversight for the Team Leaders and Principal Investigators and Project Task Leads (not shown).

Table 1. Supported Collaborating Agencies

LLNL currently supports over 300 supported and collaborating local, state, and federal organizations, including the following:

- DOE Headquarters Operations Center
- DOE Regional Operations Centers
- DOE national and international response teams
 - Accident Response Group (ARG)
 - Radiological Assistance Program (RAP) regional teams
 - Nuclear Radiological Advisory Team (NRAT), which in turn supports the Domestic Emergency Support Team (DEST)
 - Foreign Emergency Support Team (FEST)
 - Joint Technical Operations Team (JTOT)
 - Consequence Management (CM) Teams
 - Aerial Measuring System (AMS)
 - Radiological Triage, Radiation Emergency Assistance Center (REAC)
- DOE national laboratories
 - Forensic Science Center at LLNL
 - Remote Sensing Laboratory
 - Sandia National Laboratories
- DHS National and Regional Operations Centers and Response Teams
 - Homeland Security Operations Center (HSOC)
 - FEMA National Response Coordinating Center
 - FEMA Regional Response Coordination Centers
 - Transportation Security Operations Center (TSOC)
 - USCG Scientific Support Coordinators
 - US Secret Service
 - DHS Biodefense Knowledge Center (BKC) and the new National S&T Threat Awareness and Reachback (NSTTAR) at LLNL which provides 24/7 reachback for all-WMD (chemical, biological, radiological, nuclear, and explosive) assessments
 - DHS Nuclear Assessment Program (NAP) at LLNL, which provides assessments for nuclear threats, threats against nuclear reactors, cases of illicit trafficking in alleged nuclear materials, and other non-threat non-smuggling incidents
 - IMAAC interagency userbase (DHS, DoD, DOE, EPA, NASA, NOAA, NRC with HHS and DOT to be added)
- DOD National Operations Center and Teams
 - U.S. Northern Command (USNORTHCOM)
 - Defense Threat Reduction Agency (DTRA) Operations Center
 - National Guard Civil Support Teams
- EPA Operations Centers and regional On-Scene Coordinators
- NASA — Kennedy Space Center
- NOAA National Centers and Teams

- Hazardous Material Response Division
 - National Centers for Environmental Prediction (NCEP)
 - Regional Weather Forecast Offices, and Incident Meteorologists
- NRC (Nuclear Regulatory Commission) national and regional operations centers and teams
- Federal Advisory Team for Environment, Food and Health (includes EPA, USDA and HHS)
- Federal Radiological Monitoring and Assessment Center (FRMAC), which includes DHS, DOE, EPA and other federal and state agencies
- Nuclear Facilities and Sites — DOE sites, Naval Reactor sites, and DoD Sites
- Local and State Operations Centers and Teams
 - DHS Local Integration of NARAC with Cities (LINC) pilot cities New York, Cincinnati, Fort Worth, Seattle, and Albuquerque
 - 22 state emergency operations centers
 - City, county and state response organizations and operations centers
 - U.S. Capitol Police operations center

Table 2. NARAC/IMAAC Major Responses (FY2005 – Q1 FY2006)

DATE	LOCATION	RESPONSE LEVEL	MATERIAL	INCIDENT	REQUESTER
13 Oct 04	Atlanta, GA	Alert	Styrene	Train derailment	TSOC
16 Oct 04	Southern CA	Alert	Sodium hydroxide	Train derailment	TSOC
21 Oct 04	Camarillo, CA	Exercise	Cs-137, Chlorine	RDD, attack on rail car	IMAAC Director
25 Oct 04	Detroit, MI	Emergency	Methanol	Train derailment	TSOC
22 Oct 04	NYC, NY	Assessment	Anthrax	Materials Threat Assessment	DHS
13 Oct 04	Palm Desert, CA	Emergency	Germanium	Bomb threat	CST
09 Nov 04	Various, OH	Exercise	Various	Terrorist threats	LINC Cincinnati
06 Dec 04	Washington, DC	Alert	Sarin example	Threat assessment	HSOC
16 Dec 04	East Point, GA	Alert	Acetic Acid	Tank release	TSOC
06 Jan 05	Graniteville, SC	Emergency	Chlorine	Train accident	HSOC
20 Jan 05	Washington, DC	Alert	Various	SOU support	USCP
24 Jan 05	Newport, MI	Alert	Generic	Fermi 2 NPP Secondary Coolant Leak	HSOC
26 Jan 05	West Palm Beach, FL	Alert	Generic	Fire	HSOC
26 Jan 05	Bayonne, NJ	Emergency	Methyl Methacrylate	Tank release	LINC NYC
27 Jan 05	Grandview, WA	Emergency	Smoke	Fertilizer plant fire	HSOC
27 Jan 05	Washington, DC	Exercise	Cs-137	RDD	NRAT
03 Feb 05	Washington, DC	Alert	Various	SOU support	USCP
24 Feb 05	NYC, NY	Emergency	Smoke	Warehouse fire	LINC NYC
15 Mar 05	San Diego, CA	Exercise	Anthrax	BioNet Table Top Exercise	BioNet
17 Mar 05	Detroit, MI	Exercise	Cs-137	Hospital fire	NRC
05 Apr 05	New London, CT	Exercise	Mustard Gas	Terrorist attack	HSOC
27 Apr 05	Rural WA	Alert	Generic	Warehouse fire	HSOC
28 Apr 05	NTS, NV	Alert	Generic	Tornado alert	NTS
04 May 05	Thibodaux, LA	Emergency	Chlorine	Tank release	S&T Coordinator
25 May 05	San Diego, CA	Exercise	Anthrax	BioNet Command Post Exercise	BioNet
07 Jun 05	Escanada, MI	Emergency	Chlorine	Tank release	S&T Coordinator
20 Jun 05	Washington, DC	Exercise	Fission products	IND	DOE
14 Jul 05	Pantex, TX	Exercise	Rad	Pu	NIRT
15 Jul 05	Albuquerque, NM	Alert	Rad	Risk from grass fire	SNL EOC
28 Jul 05	Ft Worth, TX	Emergency	7 chemicals	Industrial facility fire	LINC Ft Worth
17 Aug 05	Ft Worth, TX	Emergency	Gasoline	Tanker spill	LINC Ft Worth
22 Aug 05	Kings Bay, GA	Exercise	Pu	Broken Arrow	SWFLANT
24 Aug 05	Hanford, WA	Alert	Pu	Waste drum spill	Hanford
30 Aug 05	Cincinnati, OH	Emergency	Styrene	Tank car spill	LINC Cincinnati
30 Aug 05	New Orleans, LA	Alert	Various	Industrial facility fire	HSOC
01 Sep 05	New Orleans, LA	Alert	Various	Industrial facility fires, tank releases	HSOC
12 Sep 05	Taylor, SC	Alert	Ethyl Acrylate	Tank release	S&T Coordinator
30 Sep 05	Washington, DC	Alert	Tularemia	BioWatch detection	S&T Coordinator
30 Sep 05	Keamey, NJ	Emergency	Chlorine	Tank release	LINC NYC
31 Oct 05	San Jose, CA	Alert	Tularemia	BioWatch detection	
15 Oct 05	Texarkana, AR	Emergency	Vinyl acetate	Railcar spill	HSOC
16 Nov 05	Wolf Creek, KS	Exercise	Mixed fission	Plume phase exercise	NRC
15 Dec 05	Salisbury, MD	Emergency	HCl	Tank release	S&T Coordinator
04 Jan 06	New Orleans, LA	Alert	Smoke	Landfill fire	EPA

Table 3. List of External Collaborators

- UC Berkeley: Fotini Chow, urban atmospheric turbulence, event reconstruction
- NCAR: Tom Warner, operational forecasting incorporating nowcasting and variational data assimilation
- NOAA/ Field Research Division: Kirk Clawson, field experiments
- NOAA Aeronomy Lab/CIRES: Wayne Angevine, boundary-layer height prediction and quantification
- University of Colorado/CIRES: Jeff Weil, turbulence and diffusion model parameterizations
- NOAA Hazardous Material Response and Assessment Division: Mark Miller, chemical hazard databases and models (CAMEO/ALOHA system)
- NRC: Stephen Mcguire, nuclear power plant accident source characteristics (RASCAL code)
- ESRI, Inc. and DOE Remote Sensing Laboratory RSL: Al Guber, Interfaces between modeling systems and GIS software
- LBNL: Ashok Gadgil / Rich Sextro, indoor exposures
- UK Defence Science and Technology Laboratory (Dstl): Ian Griffiths, Empirical urban model
- NRL: Julie Pullen and Teddy Holt, Mesoscale modeling and COAMPS
- PNNL: Jerry Allwine, Urban Dispersion Program
- LANL: Michael Brown, Urban Dispersion Program
- LANL/ORNL: Geospatial population density databases
- ORNL: Keith Eckerman, Acute and chronic radioactive dose and risk models
- SNL: John Fulton, casualty/fatality estimates and prompt effects from nuclear explosions
- SNL: Fred Harper and John Brockmann, Radiological, chemical and biological source characteristics
- U.S. Army Edgewood Chemical and Biological Center: Ray Jablonski/Doug Sommerville, Dose-response relationships and toxic load models for chemical and biological agents

Nuclear Systems Science and Engineering Program
(to be added)

Earth Systems Science and Engineering Program

Providing the essential energy and water systems to support human needs while understanding and addressing their environmental consequences is a watershed problem for the 21st century. The LLNL Earth System Science and Engineering Program seeks to provide the scientific understanding and technological expertise to help provide solutions at both global and regional scales. Our work is highly collaborative with universities, laboratories and industrial partners across the world and involves observational data, laboratory experiments, and numerical simulations.

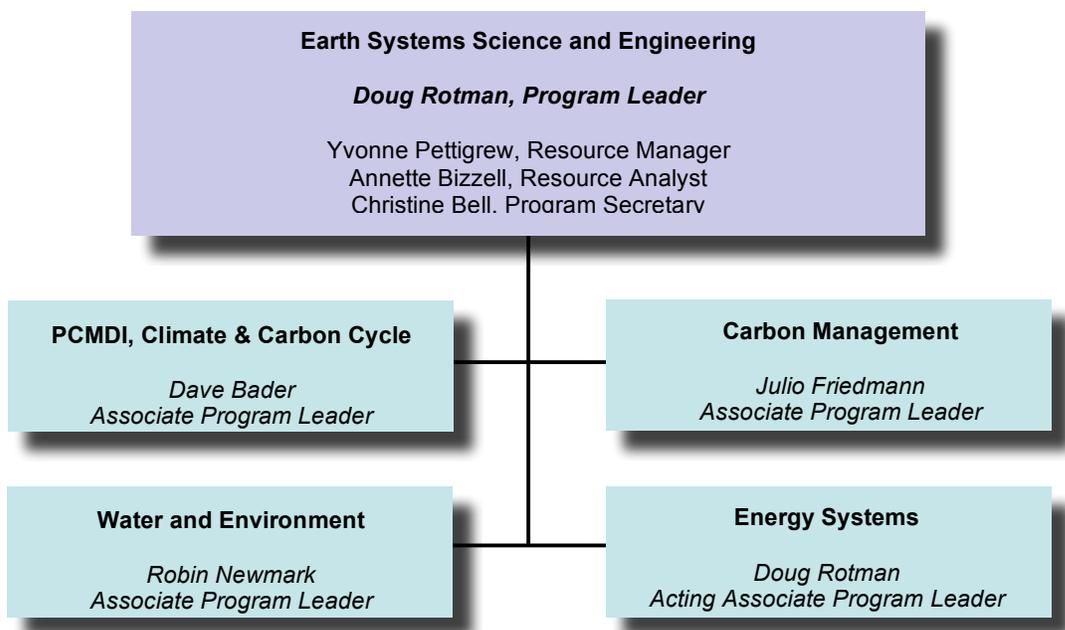
The energy systems we have enjoyed for the last 100 years have resulted in the advanced standard of living in the developed world and a major emerging problem with climate change. Now we face a simultaneous realization that our reliance on fossil fuels is a source of conflict and economic disruption as well as causing potentially abrupt, even catastrophic global climate change.

The climate and energy problem is perhaps the greatest challenge ever faced by mankind. Fossil fuel remains the least expensive and most available source of energy and the basis of our economy. The use of fossil fuels, especially over the last 100 years has led to a 30% increase in CO₂ in the atmosphere. The problem is growing. The population of the Earth will increase by several billion people in the next 50 years. If economic growth is to continue, the demand for energy is estimated to approximately double in the next 50 years so that we will need approximately 10 TW more energy than the 15 TW we use now. Much of this demand will come from the developing world where most of the population growth will occur and where advanced energy technology is not generally used.

The problem affects and is affected by a complex system of systems. The climate and energy problem will affect resources, social structure and the probability of increased conflict. No one person, no one nation, no one technology can solve the problem. There is no parallel precedent on which to model a solution. On these grounds, we have chosen to tackle four key tasks:

- Understanding the natural Earth system and anthropogenic systems examining key forcings and processes driving these systems and the interactions between systems
- Identify climate change impacts important to society and develop strategies and technologies to adapt to the climate change that is inevitable given past, current, and potential emissions
- Developing strategies and technologies to reduce/eliminate greenhouse gas emissions thereby mitigating climate change while generating energy that is economically and socially viable
- Engaging with appropriate economic, legal, social, and political structures to inform key decisions.

Over the past year, we have created and organized the Earth Systems Science and Engineering program to address these tasks; our organization is show below



These four areas compromise the foundations of our programmatic activities. Those foundations plus interactions across the four areas are critical to addressing the tasks discussed above including,

- Energy related greenhouse emissions and climate change*
- Climate change and environmental impacts (e.g. water) and adaptation strategies*
- Environmental understanding towards improved carbon sequestration*
- Carbon capture from energy systems*

The FY2006 budget of the ESSE program is \$26.8M. The distribution of this funding across the four program areas is

- PCMDI, Climate and Carbon Cycle: \$10.6M
- Carbon Management: \$1.2M
- Water and Environment: \$7.2M
- Energy Systems: \$7.8M

This budget is made up of approximately 120 projects and programs ranging in size from a few tens of thousands to nearly 5 million dollars. The vast majority of projects (~70) are peer-reviewed single PI efforts that are funded at between \$100 and \$500K. Just over 83% is DOE funding; primarily DOE Office of Science (SC), DOE Energy Efficiency and Renewable Energy (EERE) and DOE Environment, Safety, and Health (ESH). Internally funded LDRD (Laboratory Directed Research and Development) funds make

up 5% as does funding from NASA. The State of California provides 2% of our funding; we are seeking that to grow in size and impact. The remaining budget (~5%) comes from a very long list of sponsors in the federal government (DOE/FE, DOE/EM, DOD, ...) and industry – these projects are critical to the execution of the entire ESSE program.

ESSE programmatic achievements and science accomplishments depend heavily on partnerships across the national and international community. The PCMDI, almost by definition, is centered as a focal point of climate simulation analysis across the international climate community. Indeed all ESSE programs are involved with federal, state, academic and industrial partners. Over the past year we have formed especially strong relationships with UC campuses at Berkeley, Davis, San Diego, Irvine, and Merced. Additionally, aligned with a LLNL funded initiative, we have expanded our partnership with the State of California, with special focus on the California Energy Commission (CEC), Department of Water Resources (DWR), and many other organizations in the State of California. Especially within the Carbon Management program, we have also engaged in a series of industrial partnerships in individual projects as well as an industry-wide “Joint Industrial Partnership” (JIP) aimed at enabling science insight in geochemistry and geomechanics via access to LLNL computing capability.

Program Components

Carbon Management

Carbon capture and storage (CCS) has emerged as a key technology pathway to significantly reduce greenhouse gas emissions, particularly geological storage. Improved understanding of CCS economics, politics, and capture engineering has recently focused attention on the practical aspects of storage and its associated uncertainties. Concerns center on questions of risk of leakage from deep targets, both in terms of local and global risks. These concerns include both short- and long-term aspects, including direct health, safety, and environmental risks, the long-term fate of CO₂ in the subsurface, and the overall efficacy of CCS as an emissions reductions strategy. Basic scientific questions regarding the processes associated with storage, the effects of subsurface heterogeneities (both stratal and structural), and handling of risk and uncertainty remain central. Such questions continue to drive interest in monitoring, measurement, and verification technologies (MMV). MMV suites will be required in some fashion to understand subsurface processes, underpin a regulatory framework, recognize leakage before and after surface escape, and even inform financial and liability decisions on individual storage sites.

From these concerns, LLNL has chosen to focus on three primary research areas in carbon storage: numerical simulation of storage, explicit risk characterization, and improved and novel MMV techniques. We are greatly expanding our numerical modeling efforts and subsurface simulation expertise in order to better quantify and circumscribe risk aspects. This includes better geochemical and geomechanical coupling, addition of hydrocarbon and co-contaminant equations of state, and dramatic increases in computational and numerical capabilities. New output arrays will include maps and

rastor volumes that can be used for both deterministic and probabilistic risk assessments. In order to better understand the nature of potential leakage risks, we have studied natural and engineered systems to understand and constrain potential worst-case scenarios. Currently, we focus on the Crystal Geyser site in Utah, where a poorly completed well has erupted CO₂ episodically for 70 years. Our estimates of flux and concentrations suggest that this site is a good analog for well leakage large-volume storage sites. We have carried out long term measurements of CO₂ concentrations at the Crystal geyser site and are now analyzing those to assess the potential leakage consequences from this worst case scenario.

Our MMV efforts focus on two topics. The first is methods that are low-cost, non-invasive. These include electrical methods (ERT and EMIT), surface deformation records (Tilt, GPS, InSAR), other methodologies. These methods provide data that seismic methods do not, and often provide time-series information with much higher sampling rates. The second topic is integration of MMV data streams. Our preferred approach involves stochastic integration and inversion, where data streams are explicitly compared using a Monte-Carlo, Markov chain approach to Bayes theorem. We are looking at how to assess the needs of a surface monitoring array as a function of climate, population, and terrain. The goal is to construct a methodology for planning sites in a variety of settings. Initial tests have been carried out using data from an industrial CO₂ flood at Salt Creek, WY, and will expand with a new data sharing agreement with Chevron and Pinnacle Technologies Inc. Initial results with these and synthetic data sets show that new insights of subsurface carbon flows can be gained where working with individual capabilities can not attain the same results.

We have had considerable success in bringing LLNL capabilities to large scale demonstration projects in carbon sequestration. Jim Johnson has been Theme Area Coordinator for geochemistry at the Weyburn field and is currently forming a work plan and work team to continued study of the long term effects of sequestration. Julio Friedmann is chair of the technical advisory committee to CO₂SINK in Germany and serves on the FutureGen advisory committee. We hope to build on these leadership positions to additionally engage projects across the world. This year, LLNL became a member of the DOE-sponsored ZERT research consortium, and received funding to integrate results in subsurface and atmospheric modeling and risk assessment. Finally, LLNL continues to play an important role in the WestCARB regional partnership in carbon sequestration and has joined two other regional partnerships – the Southeastern partnership (SeCARB) and the Midwest partnership (Illinois Basin).

Although Carbon Management has focused on the applied science of storage, we have continued work in carbon capture and separation as well. We have continued our work in advanced membrane development using SLIP technology and formed an eight company consortium to develop a commercial platform for post-combustion capture. We have also begun new work on novel capture approaches, including a new LDRD project using desalination technology for carbon capture and combining accelerated limestone weathering with injection of co-produced water. We hope to expand this aspect of the program over the next year in partnership with DOE HQ, LANL, NETL, and non-governmental entities.

PCMDI, Climate and Carbon Cycle

The PCMDI, climate and carbon cycle program area (PCCC) seeks to answer questions of national need in climate science and the carbon cycle, with special focus on the fate of carbon in the earth system and its relationship to climate change. A strategic theme of this program is to advance our understanding of the environmental consequences from energy production/use within the context of natural variability in carbon and climate processes. Research includes global climate change and its regional ramifications, atmospheric chemistry and aerosols, atmospheric radiation and cloud physics, ocean dynamics and biogeochemistry, carbon-cycle science, climate model diagnosis and analysis, and climate change detection. PCCC carries out its research using detailed climate simulation analysis tools, high performance comprehensive climate-carbon-chemistry models, and careful linking to laboratory experiments, field campaigns, climate observations.

The PCCC anchor program is the Program for Climate Model Diagnosis and Intercomparison (PCMDI). Three other larger and DOE-driven projects are the Atmospheric Radiation Measurement (ARM) data infrastructure project, the Climate Change Prediction Program (CCPP)/ARM parameterization testbed (CAPT), and the Scientific Discovery through Advanced Computing (SciDAC) climate modeling project. The goal of the PCMDI is to collaborate with the global climate modeling community by developing standardized diagnostic methods and innovative evaluation tools to assess the scientific quality of climate simulations, thereby enabling improvements in climate model formulation and climate prediction. This program has been a primary component in the climate change research portfolio in the Office of Biological and Environmental Research (OBER) in DOE for more than a decade.

A large effort this year for PCMDI has been the archiving and data management activities for the currently working IPCC Fourth Assessment Report. PCMDI archives have housed over 60,000 files containing climate simulation results from 21 models across the climate community. All data management is handled by PCMDI and so far, they have achieved 60 Tbytes in data requests and dissemination. This data archiving and management has been done via the Earth System Grid – a data management tool developed by PCMDI in partnership with NCAR and other DOE labs. The ARM (Atmospheric Radiation Measurement) project at LLNL continues to coordinate ARM data archival and distribution as well as interacting with the Science Team in analyzing ARM data. Additionally, LLNL scientists (Steve Klein and Cathy Chuang) have become more involved in ARM science activities with funded projects in aerosol parameterizations and cloud physics along with a brand new project in partnership with other DOE labs to examine the Multi-Scale Modeling Framework (MMF) as a means to provide a more realistic representation of cloud processes and physics. The CAPT program is an innovative project of the PCMDI that ties together the diagnostic/analysis capability of the PCMDI with ARM data available via LLNL's role in data infrastructure. The idea is to initialize a climate model simulation using ARM data and to integrate the climate model in a forecast mode (i.e., short time scale). Careful examination of the climate model simulation through continued comparison to ARM data provides insight into

climate model performance. Over the past year, the CAPT testbed has completed its implementation of the AM2 climate model from the NOAA GFDL laboratory.

The Scientific Discovery through Advanced Computation (SciDAC) program at DOE is focused on a partnership with NCAR to advance the next generation of NCAR climate models. Philip CameronSmith has successfully completed simulations with a small chemical mechanism that efficiently represents the primary ozone production and loss mechanisms; analysis of the results is underway. In close collaboration with NCAR and DOE partners, we have also implemented a sulfur mechanism and carbon cycle model that enables the interactive creation of sulfate aerosols from both land based SO₂ emissions and ocean based DMS emissions as well as cycling of carbon across land-atmosphere-ocean boundaries.

To further our efforts in regional climate we have delivered to Scripps Institute for Oceanography high resolution multi-century coupled climate simulation results that will be the basis for climate change detection at regional scale. Never before has such a long and high resolution (1 degree) coupled simulation been completed. This length and resolution of simulation will allow a complete understanding of the internal modes of variability at regional scale.

Water and Environment

The Water and Environment Program (WE) area's mission is to meet the Nation's needs for science and technology to understand, secure, sustain and protect its water and environmental resources. We focus on managing the impacts of energy usage and production, defense and intelligence activities, and national security issues related to water and the environment.

Our approach includes:

- (a) Scientific research to understand and predict how natural and anthropogenic processes impacts water and environmental systems and the consequences of change.
- (b) Science and technology development to sustain water supplies to meet demand now, and in a future impacted by climate change, political and societal change, and in recognition of the health and environmental impacts of emerging contaminants.
- (c) Analytical tools and technology development to protect resources against destructive rates of use and pollution, including terrorist weapons, and to find new or better ways to monitor and treat impaired resources.

Where LLNL expertise can be of unique assistance to public agencies, industry, and academia, we seek partnerships and collaborations.

The Marshall Islands Dose Assessment and Radioecology Program provides individual and environmental measurement data and dose assessments to characterize current radiological conditions and minimize exposure of resettled and resettling populations in areas affected by U.S. nuclear testing in the Marshall Islands for DOE's Office of Health Studies. LLNL's program is accomplished through activities directed towards supporting individual radiological protection programs in whole body counting and plutonium bioassay, performing analyses on environmental samples collected during field missions, providing verification monitoring of radiological conditions in support of the resettlement program, and publishing reports or otherwise supporting DOE's informational needs in helping protect the health and safety of people living in the Marshall Islands. While the program cooperates with many institutions, the primary external collaboration is with the Joint research Center Institute for Transuranium Elements (ITU) of the European Commission; this laboratory has been providing SEM and μ XRF as well as other particle characterization studies on isolated radioactive aggregates.

This year has marked the start of a new mission in the Marshall Islands, with activities focused on the resettlement of Rongelap. LLNL's recommendations for site preparation for effective protection of human health in residential areas are being followed. The village area is being cleared, and construction has begun. Key elements of LLNL's 2005-2006 environmental missions include environmental sampling, sampling of food crop products and verification monitoring of external gamma exposure rates. A novel approach has been developed to assess potential exposure from food collections in other locations; this "pantry sampling" approach will provide information regarding the potential exposure from a key source, one with strong cultural links. Other measurements will help assess key environmental or dietary factors that could potentially change the total exposure from both internal and external sources.

WE continues to support the Energy Water Nexus activities at both the federal and state level. This effort, started under the Water Initiative, involves participation in a multi-laboratory working group, actively supporting the establishment of a DOE energy and water security program. This year, we, along with partner DOE labs, have been funded to create a roadmap articulating the national and regional needs and technology gaps, that such a program could address. The proposed national program would be in the Department of Energy and would include regional centers coupling National Laboratory and university teams dedicated to water research and technology development tasks to address the national needs described by the roadmap. On the state level, the California Energy Commission has taken steps to identify the state's water-energy relationship; LLNL staff participated in the development of the CEC's California Water-Energy Relationship Staff Paper, prepared in support of the State's 2005 Integrated Energy Policy Report (IEPR). It highlights many key issues and identifies areas for technology and policy development. Also begun under the Water Initiative, WE took a leadership role in forming a Center for Water Supply Prediction Science with support from the Association of California Water Agencies (ACWA) and lead federal, state and local

water agencies, involving the key academic researchers investigating climate change in California. On the nitrate contamination front, LLNL's Water Initiative work lead to an expansion of our role in the State's GAMA program for specific studies involving nitrate. In addition, a joint proposal (with Sustainable Conservation) addressing the application and performance verification of improved dairy management practices has been selected for funding by the State's Water Quality Control Board's Dairy Water Quality Grant Program. We have also had success in advancing the use of selective membranes for efficiently treating impaired water and seawater for desalination. Our approach combines molecular modeling and new synthesis methodologies, with promising results in developing new energy-efficient membranes for selective treatment of impaired waters. This Water Initiative-supported effort has lead to joint proposals between LLNL and industry/agencies. A project for a novel approach to desalination has been selected for funding under California's Prop. 50; another is under consideration for a hybrid approach enhancing ion exchange with electro dialysis. Our modeling codes are being applied for use in diverse applications as aligned carbon nanotubes and the design of virus detectors. The USBR has expressed interest in partnering with LLNL in part due to this work.

LLNL continues to support the Department of Interior's Bureau of Reclamation in developing an assessment of the groundwater resources in California's Imperial Valley, which may provide additional water options to consider in solving the Salton Sea–Imperial Valley water equation. Such an assessment requires the integration of a vast assortment of descriptive geologic, hydrologic, chemical, and climatic data related to the regional groundwater aquifers and the occurrence, movement, production, and quality of groundwater, with knowledge of related geologic, hydrologic, chemical, and climatic processes. For the Salton Sea area, much of this information already exists, but is in the hands of multiple public and private entities, disparate, focused on specific purposes, and often proprietary. In the first year, LLNL's team developed a database, integrating historic and recent data obtained in the region. This database is already serving to increase cooperation by different agencies, an important achievement in itself. The next steps involve developing a quantitative understanding of the key flows and fluxes in the region, and to highlight opportunities and constraints regarding use of the groundwater resource and its sustainability. This is particularly important in the East Mesa area, where significant losses from unlined canals have created a nearly century-old infiltration experiment.

WE depends on PI-driven research as the basis for successful program contributions, such as our historic strengths in fate and transport in environmental systems providing the underpinnings for our environmental management programs. EED manages the BES program in geosciences for LLNL, a program sponsored by the DOE Office of Science. The mission of this program is to develop a quantitative and predictive understanding of geologic processes related to energy and environmental quality. Reactive transport in geologic systems is the unifying theme of this research program. This subject bears on the disposal of radioactive waste, transport of contaminants, migration of hydrocarbons, and chemical evolution of the crust and mantle. The program comprises experimental programs to quantify the parameters required for tomographic observations of subsurface fluids, fundamental dissolution and precipitation kinetics and equilibria, and the geophysical theory required to invert field- based observations.

This year one investigation made a significant advance in understanding the kinetics of mineral dissolution. Dissolution rate data show apparent serious inconsistencies that cannot be explained by the largely empirical kinetic “laws.” We show that mineral dissolution can, in fact, be understood through the same mechanistic theory of nucleation developed for mineral growth. By generalizing nucleation rate equations to include dissolution, we arrive at a model that predicts how quartz dissolution processes change with undersaturation from step retreat, to defect-driven and homogeneous etch pit formation. This finding reveals that the “salt effect,” recognized almost 100 years ago, arises from a crossover in dominant nucleation mechanism to greatly increase step density. The theory also explains the dissolution kinetics of major weathering aluminosilicates, kaolinite and K-feldspar. In doing so, it provides a sensible origin of discrepancies reported for the dependence of kaolinite dissolution and growth rates on saturation state by invoking a temperature-activated transition in the nucleation process. Two new FY06 projects expand upon mineral dissolution kinetics investigating (1) the effects of aluminum in inhibiting mineral dissolution, and (2) the effects of fluid chemistry on stress corrosion cracking.

Energy Systems

The mission of the Energy Systems (ES) program area is to assure that the nation’s future energy demands can be met in an environmentally responsible manner. We will do this by:

- Increasing the efficiency of existing energy technologies while minimizing their environmental impact by optimizing energy systems and improving conversion efficiencies in engines and fuel cells
- Reducing environmental impact of existing energy technologies through improved combustion mechanisms and removal of greenhouse emissions through new fuels
- Developing new environmentally responsible technologies
- Partnering with industry to commercialize our technology

Our Homogeneous Charge Compression Engine (HCCI) activities continue to be a focal point towards improved fossil fuel combustion efficiencies with the production of fewer emissions. This technology provides a more uniform combustion of fuel via compression ignition (not via spark ignition) such that fuel mixtures and temperatures can be more completely managed and hence, NO_x emissions can be reduced. Over this year, ES has demonstrated an operational 200 kW natural gas stationary power source using HCCI technology. In doing so, Dan Flowers and Salvador Aceves have brought together a series of accomplishments over the past 2 years that have (1) implemented intake manifold design that allows for cylinder-by-cylinder temperature control, (2) developed and implemented fuel-air control for ultra-lean operation, (3) developed and demonstrated HCCI-mode startup strategy, and (4) integrated supercharger boost system. Research on this system will continue to investigate the use of different fuels.

Transportation remains a major use of fossil fuel and improving efficiencies in the transportation sector is important to reducing greenhouse gas emissions. Within the transportation sector, class 8 heavy trucks use 11% of US petroleum. Within that, 65% of the energy used is to overcome drag at highway speeds. Using LLNL's computational power and advanced Computational Fluid Dynamics (CFD) models, ES (Rose McCallen and Kambiz Salari with others) have continued to lead a consortium of DOE Labs, academia, and industries towards a goal of 25% reduction in drag. The project has identified the technologies that can obtain these goals (truck base treatments, trailer skirts, and cap splitter plates), but much more work is needed to more completely understand the physics so that less obtrusive devices can be designed and implemented.

Our research on hydrogen focuses on storage capacity and storage safety. Storage of hydrogen has various advantages such as high volumetric and gravimetric density and low adiabatic expansion energy; however, suffers from high evaporative losses and high liquefaction costs. Activities at LLNL have addressed these issues by developing and testing cryogenic pressure vessels. Cooling of hydrogen increases its safety since energy release during a sudden failure is strongly reduced at lower temperatures. Salvador Aceves and Gene Berry have lifecycle tested conventional pressure vessels at cryogenic temperatures with no loss in performance over an equivalent 200,000 miles of use. They have demonstrated flexible refueling of insulated pressure vessels in a converted truck at LLNL and completed an extended 6 month test in Palm Springs. We have just completed the purchase of a hydrogen fueled Toyota prius in which we will be testing a next generation of hydrogen storage tanks. These tanks are lighter, more compact, and are more able to conform to automobile space requirements.

For years, LLNL has led the development of a fuel cell that directly converts carbon to electricity and CO₂. The direct carbon fuel cell (DCFC) combines high conversion efficiency with a pure CO₂ stream, thus serving both as a power supply technology and a capture device. This year, LLNL has licensed the DCFC technology to Contained Energy, Inc., which is working to commercialize it. This effort includes a ~\$700k CRADA to develop an alpha prototype of a direct carbon battery.

Center for Accelerator Mass Spectrometry

Program Leader – John Knezovich

Background

The Center for Accelerator Mass Spectrometry (CAMS) operates as an institutional science facility that develops and applies state-of-the-art ion-beam analytical techniques to a broad spectrum of scientific disciplines. Dissemination of AMS technology, coupled to the needs of scientific users, is an appropriate mission for LLNL and is of special value to the Laboratory's University Relations Program. Advances in spectrometer hardware coupled with an operational philosophy of around-the-clock operation have made CAMS the most versatile and productive facility of its kind in the world. At this time, CAMS scientists are focused on advancing the applications of ion-beam techniques to biomedical sciences, creating sustainable significant contributions to earth and environmental sciences, and developing and applying AMS and accelerator capabilities for national security applications. Support for these activities comes from the LLNL University Relations Program, DOE, DoD, NIH, NSF, FBI, CIA, and from contracts with more than 70 commercial sponsors and university collaborators.

CAMS maintains three accelerators in B190, dedicated to nuclear microprobe studies, biomedical studies, and general AMS and ion-implantation work. The latter uses the largest of the three accelerators, the High Voltage Engineering Corporation Model FN Tandem Van de Graaff. AMS is a sensitive technique for the detection and quantification of numerous long-lived radioisotopes.

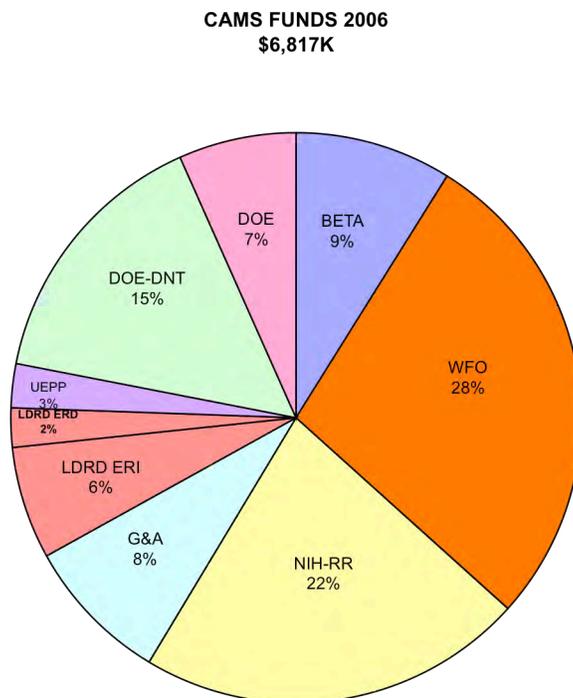
The 1-MV AMS system supports biomedical research using ^{14}C -labeled compounds. This spectrometer is the core component of the National Research Resource grant awarded by the NIH. It has significantly increased capacity for ^{14}C -labeled biological samples while serving as a test bed for advanced sample preparation and delivery technologies. Work is under way to add a second source to this system for tritium and gas-ion analyses.

The CAMS nuclear microprobe is a versatile instrument that is being applied to a variety of environmental and biomedical research projects. This instrument, when used in the proton-induced x-ray emission (PIXE) mode, has the capability to perform elemental mapping of substances at a resolution of one micron. This capability has been particularly useful for defining the processes by which metals transit the blood-brain barrier. In addition, this system is being used to characterize isolated proteins and interstellar particles as part of NASA's Stardust mission.

Budget

CAMS has an expected budget of approximately \$6.8M during 2006 (Figure 1). The budget consists of work-for-other research and service, research and infrastructure support from DOE, LDRD, and institutional investments in facility operation and

upgrades (see below). This budget profile does not include funds for projects in other directorates in which CAMS staff participate through the LLNL matrix system (e.g., microprobe analyses for the NASA Stardust mission, target characterization for NIF).



Center for Accelerator Mass Spectrometry expected funding for FY06 (NIH RR = National Institutes of Health Research Resource, DOE = Department of Energy, DOE/DNT = DOE funded programs through the Defense & Nuclear Technologies directorate, BETA = contract with BETA Analytic, WFO = work for others (>70 contracts), LDRD ERI = Laboratory Directed R&D Exploratory Research in the Institutes, IGPE = institutional general purpose equipment, G&A = general and administrative).

Significant Accomplishments

CAMS scientists, in collaboration with the Biology and Biotechnology Research Program, successfully defended the renewal of their NIH-funded National Research Resource for Biomedical AMS. This resource is a national focal point for AMS research with the university community. The original grant, which has been funded since 1999, focused on establishing a dedicated AMS system at CAMS for biomedical research using ^{14}C and for developing a broad set of collaborative research projects. The renewal proposal is focused on developing methods for single-cell AMS, innovative methods for post-labeling, and the addition of tritium AMS as a routine analytical capability. In their assessment of the project renewal, the NIH site visit team stated: “This application proposes innovative approaches to significant biomedical problems to be performed by a highly accomplished team.” As a national resource that develops and provides cutting

edge technology to the biomedical research community, the review team concluded: “Service, training and dissemination were viewed as exceptional.” The renewed grant will be funded at a level of \$8M over a period of five years.

In September of 2005, CAMS organized the 10th International Conference on Accelerator Mass Spectrometry. This conference, which is held once every three years, attracted over 300 scientists from 26 countries. The proceedings of this conference, which are being edited by CAMS staff, will be published as a special volume of *Nuclear Instruments & Methods* in 2006.

In 2004 CAMS research was featured on the covers of 3 journals (*Environmental Science & Technology*, *Geology*, *Meteoritics & Planetary Science*). In 2005, CAMS research was featured on the covers of 3 additional journals:

- *Cell* (**122**: 133): Retrospective Birth Dating of Cells in Humans.
- *Nature* (**436**: 538): Young Organic Matter as a Source of Carbon Dioxide Outgassing from Amazonian Rivers.
- *Clinical Chemistry* (**51**/118: 2095): ⁴¹Ca and the Evaluation of Clinical Bone Biology

Routine measurement of actinides at micro-becquerel levels is now routine and is being used to reconstruct exposure in humans. Measurements of ¹²⁹I have been demonstrated and are enabling groundwater characterization.

Infrastructure Investments

The future success of CAMS as an institutional science facility will require continual advancements of capability in order to meet and drive the needs of sponsors. During the past year, five projects were initiated that are significantly increasing CAMS’ capabilities:

1. High-precision ¹⁴C

Last year, CAMS scientists demonstrated ±1 per mil measurement precision for ¹⁴C—an unheard-of level of precision in the AMS community. This achievement will enable the assessment of CO₂ budgets on a regional scale and the determination of fluxes between the atmosphere and ocean. In FY05 CAMS received \$445K of capital equipment funds from DOE’s Office of Biological and Environmental Research (OBER) to build a new ion source for the 10-MV AMS system. This new ion source and associated injection magnet will enable high-precision (i.e., 1 per mil) ¹⁴C measurements at increased throughput. To date, the new magnet has been installed and is operational. Once completed, this capability will enable regional assessments of carbon budgets and will increase the throughput for other AMS isotopes.

2. Gas Ion Source

The Laboratory's Genomes to Life (GtL) scientific planning committee has identified the need for advanced methods for analysis of single cells. To help meet this need, CAMS has received \$600K of institutional funds (G&A and IGPE) to date to optimize and bring to routine practice a gas-ion source that is being added to the CAMS 1-MV AMS system. The online conversion of a sample to CO₂ gas with the CO₂ fed directly into an ion source for trace isotope analysis is required for ultimate sensitivity. This capability will enable the Laboratory to meet immediate needs of current programs (i.e., the NIH Research Resource for BioAMS) as well as DOE's emerging GtL Program.

3. Proton Tomography Capability

A high-energy ion microprobe to enable micron-scale proton tomography of mesoscale objects would be an asset to the Engineering directorate's x-ray imaging of mesoscale objects. CAMS received \$275K of institutional funds (G&A and LDRD) to retrofit a beamline for proton tomography on the CAMS 10-MV accelerator. This capability is now on-line and we plan to characterize the HEDP and other mesoscale reference standards developed by engineering and elsewhere to benchmark protons and compare the advantages and disadvantages of proton imaging with x-rays, acoustics and MRI measurements performed on the same bench-marked standards. This capability will ultimately support the characterization of NIF targets.

4. Nuclear Microprobe Upgrades

The CAMS nuclear microprobe is undergoing a variety of upgrades to meet emerging program needs: (1) upgrades to imaging slits have been provided by Sandia National Laboratory; (2) a Hadamard TOF-MS spectrometer that enables the detection of molecular fragments was purchased with \$60K from DOE/NA-22; (3) UV/VIS and near-infrared spectrometers were obtained with LDRD funds; and (4) a time-of-flight STIM detector (\$41K) and an enhanced x-ray detector (\$68K) were purchased with NASA funds. The last two items were installed in anticipation of performing analyses on interstellar particles that returned to earth in January, 2006 as part of NASA's Stardust mission.

5. Helium-ion implantation Capability

A fundamental issue in nuclear power and weapons is the behavior of the materials with aging due to their radiolytic environment. Aging effects can generate several percent swelling during the lifetime of the component and even stronger effects in strength and other properties. Fissile materials swell due to hundred kilovolt heavy ion recoils from the ongoing alpha decay that is primarily known for its release of megavolt energy helium ions. These two processes in self-irradiation cause void formation from the recoils and helium bubble formation from the stopped helium ions. Study of these effects is hindered by the difficulty of handling radioactive samples, and the paucity of aged specimens with well-documented microstructure.

To generate aged samples with an equivalent amount of helium produced from up to 250 years of decay, Helium-ion implantation into materials will be performed at CAMS. To enable such work, CAMS is developing a high energy, high current helium implantation

capability on the 10-MV FN accelerator. No facilities are better suited than CAMS accelerator facility for the high beam energies, beam stability and fluxes required. Samples with as much as 1 atom percent Helium and 200 microns thick will be fabricated in an even, minimally perturbing fashion. Creation of these implanted samples would produce material of great value for determining the behavior of aged materials. The Defense and Nuclear Technologies directorate has obligated \$1,050K of funds from the Stockpile Stewardship Program to develop this capability in FY06.

This capability can also be used to great advantage in simulating radiation fields that would exist in nuclear power stations. Contrary to samples aged in a nuclear reactor, samples aged by ion-beams do not become radioactive. Moreover, years of simulated ageing can be accomplished with a few days of ion-beam irradiation. Because many accelerators have been shut down in the U.S., CAMS is becoming one of the last resources for such important capabilities.

Overall, these technical improvements will enable scientific advances (e.g., understanding regional carbon dynamics, metabolic function at the cellular level) while increasing the ability to address national security needs. To achieve these goals, CAMS will continue to rely on a strong multidisciplinary staff, collaborative relationships within the Laboratory, and effective partnering with the academic scientific community.

Significant CAMS Collaborations (2005)

- UC Berkeley (Bruce Ames, Michael Manga, Whendee Silver)
- UC Davis (Andrew Clifford, Jason Eiserich, Bruce Hammock, Su-Ju Lin, Yumei Lin, Krishnan Nambiar)
- UC Irvine (John Southon, Susan Trumbore)
- UC Merced (Sam Traina, Martha Conklin)
- UC San Diego (Lihini Aluwihare, Ralph Keeling, Robert Fitzgerald)
- UC Santa Cruz (Paul Koch, Matthew McCarthy)
- Albert Einstein College of Medicine (Vern Schramm)
- Karolinska Institute (Kirsty Spalding)
- Lamont Doherty (Peter deMenocal)
- Oregon State University (Beverly Law)
- Stanford (Daria Mochly-Rosen, Richard Zare)
- University of Illinois (Feng Sheng Hu)
- University of Leicester (Karen Brown)
- University of New Mexico (Johnnie Lewis)
- University of Texas (Steven Biegalski)
- University of Utah (Cynthia Burrows)
- University of Vermont (Paul Bierman)
- University of Washington (John Stone, Jay Heinecke)

- University of Wisconsin (Hector DeLuca)
- LBNL (Margaret Torn)
- ORNL (Paul Hanson, Phil Jardine)

Acronyms

AD	Associate Director
ADCFMI	Atmospheric Dispersion and Consequences Management Initiative
AFTAC	Air Force Technical Applications Center
AGG	Applied Geology and Geophysics
AGU	American Geophysical union
AMIP	Atmospheric Model Intercomparison Project
AMS	accelerator mass spectrometry
ANL	Argonne National Laboratory
ANS	American Nuclear Society
ANSI	American National Standards Institute
ARAC	Atmospheric Release Advisory Center
ARAP	Atmospheric Release Assessment Program
ARICE	Advanced Reciprocating Internal Combustion Engine
ARM	atmospheric radiation measurement
ASCI	Accelerated Strategic Computing Initiative
ASD	Atmospheric Science Division
ASME	American Society of Mechanical Engineers
ASTM	American Society of Testing and Materials
BER	Biological and Environmental Research
BES	Basic Energy Sciences
BNL	Brookhaven National Laboratory
BSC	Bechtel SAIC
Caltrans	California Department of Transportation
CAMS	Center for Accelerator Mass Spectrometry
CAPS	Counterproliferation Analysis and Planning System
CAPT	CCPP-ARM Parameterization Testbed
CASC	Center for Applied Scientific Computing
CBNP	Chemical and Biological National Security Program
CCPP	Climate Change Prediction Program
CCRI	Climate Change Research Initiative
CCSM	Community Climate Systems Model
CCSP	Climate Change Science Program
CDAT	Climate Data Analysis Tools
CEC	California Energy Commission
CENTCOM	U.S. Central Command
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act (U.S. EPA)
CFD	computational fluid dynamics
CFR	Code of Federal Regulations
CLC	Campus-Laboratory Collaboration
CMCC	Carbon Management and Climate Change

CMIP	Coupled Model Intercomparison Project
CMS	Chemistry and Materials Science
CO ₂	carbon dioxide
COTS	commercial off-the-shelf
CRADA	Cooperative Research and Development Agreement
CW	chemical weapon(s)
DARPA	Defense Advanced Research Projects Agency
DELTA	Detection and Evaluation of Long-Range Transport of Aerosols
DHS	U.S. Department of Homeland Security
DNAPL	dense non-aqueous phase liquids
DNT	Defense and Nuclear Technology
DOC	U.S. Department of Commerce
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
DST	Drift Scale Test
DTRA	Defense Threat Reduction Agency
E&ED	Energy and Environment Directorate
EERE	Energy Efficiency and Renewable Energy
EBS	Engineered Barrier System
EMSP	Environmental Management Science Program
EOR	enhanced oil recovery
EPA	Environmental Protection Agency
EPD	Environmental Control Department
EPRI	Electric Power Research Institute
ERT	electrical resistance tomography
ESG	Earth System Grid
ES&H	environment, safety, and health
ESTCP	Environmental Security Technology Certification Program
ETD	Energy Technology Division
ETSP	Energy Technology and Security Program
FE	Fossil energy
FSC	Forensic Science Center
FTE	full-time equivalent
G&A	general and administrative
GFDL	Geophysical Fluid Dynamics Laboratory
GIS	Geographical Information Science
GMI	Global Modeling Initiative
GNEM	Ground-based Nuclear Explosion Monitoring
HC	Hazards Control
HCCI	Homogeneous Charge Compression Ignition

HEFP	Hazards, Energy, and Field programs
HEU	highly enriched uranium
HMC	Hazard Mitigation Center
IGPE	institutional general purpose equipment
IGPP	Institute of Geophysics and Planetary Physics
IMPACT	Integrated Massively Parallel Chemistry and Transport model
INCCA	INtegrated Climate and CARbon
INEEL	Idaho National Engineering and Environmental Laboratory
IPCC	Intergovernmental Panel on Climate Change
IRCCSI	Institute for Research on Climate Change and Its Societal Impacts
IRIS	Incorporated Research Institutes for Seismology
ISM	Integrated Safety Management
ISSM	Integrated Safeguards and Security Management
JAERI	Japan Atomic Energy Research Institute
LA	License Application
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LC-MS	liquid chromatography-mass spectrometer
LDRD	Laboratory Directed Research and Development
LDRD-ER	LDRD Exploratory Research
LDRD-LW	LDRD Laboratory-Wide
LDRD-SI	LDRD Strategic Initiative
LEU	low enriched uranium
LLNL	Lawrence Livermore National Laboratory
LMEC	Laboratory for Mechanistic Environmental Chemistry
LSTO	Laboratory Science and Technology Office
M&IC	Multiprogrammatic and Institutional Computing
MIT	Massachusetts Institute of Technology
NAI	Nonproliferation, Arms Control, and International Security
NARAC	National Atmospheric Release Advisory Center
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCCTI	National Climate Change Technology Initiative
NCDC	National Climate Data Sensor
NE	Nuclear energy
NETL	National Energy Technology Laboratory
NFE	near-field environment
NGASE	Natural Gas Assisted Steam Electrolyzer
NGOTP	Natural Gas and Oil Technology Partnership
NIF	National Ignition Facility
NIH	National Institutes of Health

NIST	National Institute of Standards and Technology
NMSSUP	Nuclear Material Safeguards and Security Upgrade Project
NNSA	National Nuclear Security Administration
NOAA	National Oceanic and Atmospheric Administration
NRC	Nuclear Regulatory Commission
NREL	National Renewable Energy Laboratory
NRL	Naval Research Laboratory
NSF	National Science Foundation
NSPS	Nuclear Site Protection System
NSWC	Naval Surface Warfare Center
NTS	Nevada Test Site
NTSS	Nuclear Technology and System Safety
OBER	Office of Basic Energy Research
OCRWM	Office of Civilian Radioactive Waste Management
OPC	organizational personnel costs
ORNL	Oak Ridge National Laboratory
OSHA	Occupational Safety and Health Administration
OSTI	Office of Scientific and Technical Information
PAT	Physics and Advanced Technologies
PBPK	pharmacokinetic
PCM	Parallel Climate Model
PCMDI	Program for Climate Model Diagnosis and Intercomparison
PI	principal investigator
PIXE	proton-induced x-ray emission
PM	Performance Measure
PNNL	Pacific Northwest National Laboratory
PRT	professional research and teaching
P&TSP	Packaging and Transportation Safety Program
RAM	radioactive material
R&D	research and development
RCRA	Resource Conservation and Recovery Act (U.S. EPA)
ROA	Research Opportunity Announcement
RRM	Risk and Response Management
RSTR	Remote Sensor Test Range
SAIC	Science Applications International Corporation
SARP	Safety Analysis Report for Packaging
SAT	Security and Automation Technologies
SBIR	Small Business Research Initiative
SCEC	Southern California Earthquake Center
SciDAC	Scientific Discover through Advanced Computing
SERDP	Strategic Environmental Research and Development Program
SF&T	Subsurface Flow and Transport

SNL	Sandia National Laboratories
SOFC	solid oxide fuel cell
SR	Site Recommendation
SRS	Savannah River Site
SSEC	Safeguards and Security Engineering Computations
S&T	science and technology
SUNY	State University of New York
THMC	thermal-hydrologic-mechanical-chemical
TIP	Transparency Implementation Program
TMDL	total maximum daily load
UAE	United Arab Emirates
UC	University of California
UGAPS	Underground Analysis and Planning System
UGTA	Underground Test Area
UK	United Kingdom
USGS	U.S. Geological Survey
USN	U.S. Navy
VOCs	volatile organic compounds
VZO	Vadose Zone Observatory
WMD	weapon(s) of mass destruction
WMO	World Meteorological Organization
YMP	Yucca Mountain Program
ZEST	Zero Emission Steam Technology

Appendices

Appendix A: Publications

Appendix B: Contract 48 Performance Objectives

Appendix F—Standards of Performance

Modification No. M540, Supplemental Agreement to Contract No. W-7405-ENG-48

PREAMBLE

The following Standards of Performance consist of Strategic Performance Objectives and supporting Performance Measures and are the primary components of the performance-based management system described in the Section H clause entitled Performance-Based Management.

Implementation of this Appendix is supported by the Contractor's Evaluation Plan (CEP) that includes implementation guidelines for each Performance Measure. These guidelines establish points of accountability and include procedures for addressing Level 2 budget planning milestones. Where appropriate, performance targets and related dates for each measure should be addressed. The Contractor will be responsible for working with NNSA HQ Program Managers to correlate all Level 1 and 2 milestones to one or more corresponding Appendix F Performance Measures. The result of this correlation shall be included as part of the implementation guidelines. Evaluation of Contractor performance shall include evaluation of performance on all of the associated Level 1 and 2 milestones.

The Parties agree that the LSO Site Office Manager, UCOP, and the Laboratory Director will jointly review the CEP's implementation guidelines for the purpose of obtaining NNSA comment and input. The Site Office Manager will collect and summarize the NNSA input on the Contractor's CEP implementation guidelines and communicate the input to the Contractor as appropriate. It is the intent of the Parties that issues involving the CEP implementation guidelines will be resolved to the maximum possible extent and that unresolved issues, if any, will be included in NNSA's annual Performance Evaluation Report.

LLNL performance in support of Stockpile Stewardship should include its cooperation and collaboration efforts with the other Nuclear Weapons Complex sites. In order to ensure a smooth transition from the existing LANL prime contract to the FY 2006 contract, UC will work to ensure continuous cooperation between the two Laboratories.

Performance Area: Mission

Performance Objective # 1: Conduct warhead certification and assessment actions using the Quantification of Margins and Uncertainties (QMU) methodology.

Performance Measures:

- 1.1 Use progress toward quantifying margins and uncertainties, and experience in application to further refine and document a common certification/assessment methodology with Los Alamos National Laboratory.
- 1.2 Demonstrate application of the common certification/assessment methodology, (QMU) in major warhead assessments and the certification of Life Extension Program (LEP) warheads.
- 1.3 Complete the annual assessments of the safety, reliability, and performance of all warhead types in the stockpile, including conclusions on whether nuclear testing is required for resolution of any issue, the adequacy of Stockpile Stewardship tools, and other issues as required by law. Support NNSA as required during interagency and community coordination of the Annual Assessment Process.

Performance Objective # 2: Develop with NNSA and implement long-term, balanced, integrated stewardship.

Performance Measures:

- 2.1 Support the needs of warhead assessment, certification, and simulation validation by executing a coordinated program of targeted small- and large-scale experiments and mining of archival UGT data to improve predictive capability. In cooperation with LANL, develop and execute a program of hydrotests and subcritical experiments that addresses assessment and certification needs.
- 2.2 Conduct design and analysis of nuclear weapons that address the future needs of the U.S. nuclear deterrent.
- 2.3 Develop and demonstrate Science Campaign models, experiments, and capabilities that support the ongoing needs of stockpile assessment and certification.
- 2.4 Develop and demonstrate Advanced Simulation Computing (ASC) capabilities that support the ongoing needs of stockpile assessment and certification.
- 2.5 Improve and apply tools and models for prediction of systems, subsystems, and/or component lifetimes. By the end of FY 2006, determine a technically defensible estimate of the pit lifetime for the primary of each of the weapons systems for which LLNL is responsible.

- 2.6 Develop and implement a collaborative and complementary program of experiments at High Energy Density (HED) facilities that supports assessment and certification needs.
- 2.7 Develop, implement, and lead an integrated national program (National Ignition Campaign (NIC)) with the goal to achieve ignition at NIF in 2010.
- 2.8 In cooperation with LANL and NNSA HQ, continue the development and implementation of an integrated program and governance model for plutonium capabilities of LANL and LLNL to support the overall NNSA strategic requirements.
- 2.9 In support of Responsive Infrastructure (RI), develop and execute projects to improve the responsiveness of the design, manufacturing, and testing infrastructure of the integrated nuclear weapons complex.

Performance Objective # 3: Develop with NNSA and implement near-term balanced weapon programs that are coordinated with the other NNSA M&O site contractors and DoD customers and that foster complex-wide solutions to meet the needs of the U.S. nuclear deterrent.

Performance Measures:

- 3.1 Conduct stockpile surveillance activities, investigate significant findings and issues identified in technical assessment reports on a prioritized basis, and establish closure plans for Significant Finding Investigations (SFIs).
- 3.2 Deliver on the major milestones for the LEP for the W80-3 in accordance with the joint DOE/DoD phase 6.x process. Continue to support LANL on the LEPs for the W-76 and the B61-7/11.
- 3.3 Deliver on Pit Manufacturing and Certification Project major milestones.
- 3.4 Meet directive schedule requirements.
- 3.5 Provide technical support to production complex operations, including the Integrated Weapons Activity Plan (IWAP), the weapons point of contact programs, and weapons response analyses.
- 3.6 Continue to implement and execute, in accordance with NNSA-approved plans, a weapons design and manufacturing quality assurance program consistent with NNSA requirements (QC-1, Rev 10).

- 3.7 Develop and implement streamlined, multi-site, technical business practices with other Nuclear Weapons Complex partners.

Performance Objective # 4: Implement an integrated science- and technology-based program aimed at preventing the proliferation or terrorist acquisition of weapons of mass destruction as well as detecting and responding to their deployment or use.

Performance Measures:

- 4.1 Provide technical capabilities to limit or prevent the spread of materials, technology, and expertise relating to weapons of mass destruction (WMD); eliminate or secure inventories of surplus materials and infrastructure usable for nuclear weapons; and enable the implementation of U.S. nonproliferation policy.
- 4.2 Provide scientific research capability that produces cutting-edge R&D as well as the testing and evaluation needed to detect, identify, and monitor proliferation and terrorist-related WMD activities.
- 4.3 Support the needs of the intelligence community by providing intelligence analysis capabilities and science and technology that improve the nation's ability to detect and thwart proliferation and terrorism.
- 4.4 Develop and support the deployment of technologies and analytical capabilities that strengthen the nation's ability to protect against and respond to terrorist use of WMD and other threats against the U.S. homeland.
- 4.5 Apply advanced science and technology to meet immediate and long-term U.S. defense community needs.
- 4.6 Maintain and deploy, as required, nuclear emergency response teams for CONUS and OCONUS response to radiological and nuclear threats.

Performance Objective # 5: Enhance and nurture a strong science, engineering, and technology base in support of national security strategic objectives.

Performance Measures:

- 5.1 Nurture and maintain the Laboratory science and engineering excellence in disciplines and capabilities needed to support our national security missions and emerging national needs.
- 5.2 Develop and implement an integrated and balanced strategy for investing LDRD, programmatic and institutional resources to ensure the long-term vitality of the Laboratory science, engineering, and technology base in support of national security missions and emerging national needs.
- 5.3 Execute non-NNSA sponsored projects and programs that make use of the Laboratory's unique expertise, capabilities, and facilities; and that enhance the Laboratory's ability to accomplish its current and future national security missions, including those related to homeland security and homeland defense.
- 5.4 Foster active participation in the broad scientific and technical community, leveraging unique Laboratory expertise and capabilities; develop strategic collaborations with other national laboratories, industry, and academia.

Performance Objective # 6: Optimize current and evolving mission performance by providing effective and efficient facilities and infrastructure.

Performance Measures:

- 6.1 Operate mission essential and user facilities as national capabilities, including National Ignition Facility, Device Assembly Facility, Superblock, Site 300, and High Performance ASC Computers.
- 6.2 Execute construction projects as identified and agreed between NNSA and the Laboratories within scope, schedule, and budget; and develop and implement a site-wide Earned Value Management System (EVMS), and have that system certified by an independent auditor.
- 6.3 Improve and sustain the physical infrastructure needed to support Laboratory operations.
 - Execute the Facilities and Infrastructure Recapitalization Program.
 - Manage facilities in a manner consistent with NNSA's deferred maintenance goals and other objectives as stated in the approved Ten-Year Comprehensive Site Plan.
 - Sustain planned availability of mission essential facilities.
 - Implement the FY06 NNSA-approved Maintenance Implementation Plan (MIP).

- Maintain 2%+ maintenance funding relative to Real Property Value for FY 2007.
- 6.4 Support planning, implementation, and execution of special nuclear material (SNM) consolidation and/or relocation activities, including reducing inventories of surplus and excess SNM consistent with DOE/NNSA approved plans.

Performance Area: Operations

Performance Objective # 7: Utilize UC strengths to recruit, maintain, and develop the workforce.

Performance Measures:

- 7.1 Maintain a skilled and diverse workforce that meets the Laboratory's long-range core and critical skills requirements by implementing a human resource strategy that leverages student programs and UC relationships.
- 7.2 Develop an institutional plan to manage the Defense Program's full-time-equivalent reductions as specified in the "Defense Programs FY 2007 to FY 2011 Program and Resource Guidance," dated March 4, 2005.
- 7.3 Sustain leadership and management development programs that achieve workforce and diversity objectives.

Performance Objective # 8: Maintain safe, secure, environmentally sound, effective, and efficient operations in support of mission objectives.

Performance Measures:

- 8.1 Achieve continuous improvement in Integrated Safety Management System performance:
 - Assure consistent and effective application of ISM principles across all organization levels and across all Laboratory facilities.
 - Ensure effective implementation of an ES&H corrective action management program, including institutional corrective actions derived from violations enforceable under the Price Anderson Amendments Act.
- 8.2 Improve the following programs within the criteria identified:
 - The Institutional Contractor System Engineer Program within the NNSA-approved schedules.
 - An Emergency Management Program within the NNSA-approved schedules in the Emergency Readiness Action Plan (ERAP).
 - The relevant configuration management program tasks identified for implementation this year.
- 8.3 Comply with and achieve continuous improvement in nuclear safety and quality performance under 10 CFR 830 for both LLNL and LLNL operations at the Nevada Test Site.
 - Implement the Building 332 Documented Safety Analyses and Technical Safety Requirements within the NNSA-approved schedules.

- Implement the Unreviewed Safety Question process site wide within the NNSA-approved schedules.
 - Resume operations in Building 332 within the NNSA-approved schedules.
- 8.4 Maintain an environmental management program consistent with the DOE-approved baseline, funding levels, policy, and negotiated regulatory requirements.
- Demonstrate performance of the ISO 14001 Environmental Management System.
 - Effectively manage the direct funded environmental restoration and waste management programs, including environmental compliance agreements.
- 8.5 Achieve continuous improvement in security performance through ISSM and risk management principles.
- Demonstrate continuous improvement in the implementation of ISSM including line management directed self-assessments.
 - Develop and implement appropriate plans and initiatives in accordance with DOE/NNSA policies so that NNSA expectations are addressed while balancing mission requirements with S&S resource allocations and new requirements.
 - Effectively manage accountable Classified Removable Electronic Media (CREM).
 - Effectively account for Special Nuclear Materials.
 - Implement corrective actions as a result of findings from external agencies in accordance with the approved timeline in the corrective action plan.
- 8.6 Detect, deter, and mitigate foreign intelligence collection and espionage and international terrorist threats.

Performance Objective # 9: Improve or maintain effective business processes and systems that safeguard public assets and support mission objectives.

Performance Measures:

- 9.1 Demonstrate effective internal business controls and processes to maintain acceptable Financial Management and Human Resources systems and approved Procurement, Personal Property Management, and Litigation Management systems. This includes the management of a risk-based, cross-functional, integrated, and credible assessment program.
- 9.2 Demonstrate continuous improvement in the effectiveness of business processes and the information technologies that support these business systems (i.e., Financial Management, Human Resources, Procurement, Personal Property Management, and Information Management).

- 9.3 Demonstrate improvement in cost effectiveness of both institutional processes and management systems.
- 9.4 Demonstrate an effective integrated monitoring program that documents and tracks corrective actions and which addresses all internal and external business system review findings and recommendations.

Performance Objective # 10: Sustain and/or implement effective Community Initiatives.

Performance Measures:

- 10.1 Leveraging the UC expertise and mission in science education, the laboratories will establish and maintain science education outreach programs with the joint goals of community outreach and substantive contribution to science education.
- 10.2 The Laboratory will develop local community initiatives to include those programs or responses addressing mutual goals and concerns.

**FISCAL YEAR 2006
PERFORMANCE EVALUATION PLAN
ADJECTIVAL RATING**

Performance Evaluation Category	Adjectival Description and Rating			
	Outstanding	Good	Satisfactory	Unsatisfactory
<i>Mission:</i> Overall Performance	Clear evidence of the highest level of performance in most areas that would be ranked as “best in class” or comparable to the highest performing peers.	Clear evidence of a high level of performance in most areas that is comparable to high performing peers.	Performance is comparable to average performing peer groups.	Performance in most areas is significantly below average performing peer groups.
<i>Mission:</i> Performance Against Milestones	Work exceeds negotiated customer expectations in most areas (for work under change control, completed ahead of schedule and within budget).	Work exceeds negotiated customer expectations in many areas (for work under change control, some areas are completed ahead of schedule and within budget).	Work meets negotiated customer expectations in most areas (for work under change control, most work done on schedule and within budget but some may have been completed with documented failures to keep to schedule or budget).	Work does not meet negotiated customer expectations in most areas (for work under change control, performance causes substantive delays toward completion, significant schedule lapses, or large budget overruns for important programmatic activities).
<i>Mission:</i> Need for Improvement	Performance in all areas is at least at a high level.	While there may be need for improvement in some elements, overall performance in the mission areas is at a high level.	There may be need for improvement in some elements – deficiencies do not substantively affect overall performance.	Deficiencies are serious, and may affect overall performance. Prompt corrective action is required in most areas with immediate senior management attention.
<i>Mission:</i> Sustainability	Work is performed in a manner that strengthens the institution, builds core competencies, and contributes to its longer-term vigor.	Work was done in a manner that benefits the institution’s scientific capability and contributes to the quality of science.	Work maintains but does not add to the institution’s capability. Management attention is needed to rise to the next level of performance.	Performance reflects poor quality of science and weakens the institution.
<i>Mission:</i> Evaluation/Improvement Process ¹	A fact-based, systematic evaluation and improvement process is in place and implemented for most areas.	The beginning of a systematic approach to evaluation and improvement in most areas is evident.	Early stages of a transition from reacting to problems to a systematic evaluation process and a general improvement orientation are evident.	Little evidence of a systematic evaluation process or an improvement orientation; improvement is achieved through reacting to problems.

¹The rating will consider the results achieved and the level of improvement achieved by the contractor. This will be accomplished by utilizing the methodology above

Performance Evaluation Category	Adjectival Description and Rating			
	Outstanding	Good	Satisfactory	Unsatisfactory
Operations: Overall Performance	Significantly exceeds the operational performance expectations including tasks and deliverables.	Exceeds the operational performance expectations including tasks and deliverables.	Meets the operational performance expectations including tasks and deliverables.	Significantly below the operational performance expectations including tasks and deliverables.
Operations: Performance Against Milestones	Work exceeds the negotiated customer expectations in most areas (for work under change control, completed ahead of or on schedule and within budget).	Work exceeds the negotiated customer expectations in many areas (for work under change control, some areas are completed ahead of schedule and within budget).	Work meets the negotiated customer expectations in most areas (for work under change control, most work done on schedule and within budget but some may have been completed with documented failures to keep to schedule or budget).	Work does not meet negotiated customer expectations in most areas (for work under change control, performance causes substantive delays toward completion, significant schedule lapses, or large budget overruns for important programmatic or operations activities.)
Operations: Need for Improvement	Performance in all operational areas is at least at a high level.	While there may be need for improvement in some elements, overall performance in operational elements is at a high level.	There may be need for improvement in some elements, -deficiencies do not substantively affect overall performance	Deficiencies are serious and may affect performance in other areas and overall mission results or result in serious safety, security, or business problems. Prompt corrective action is required in most areas with immediate senior management attention.
Operations: Evaluation/ Improvement Process ¹	A fact-based, systematic evaluation and improvement process is in place and implemented for most areas.	The beginning of a systematic approach to evaluation and improvement in many areas is evident.	Early stages of a transition from reacting to problems to a systematic evaluation process and a general improvement orientation are evident.	Little evidence of a systematic evaluation process or an improvement orientation; improvement is achieved through reacting to problems.

¹The rating will consider the results achieved and the level of improvement achieved by the contractor. This will be accomplished by utilizing the methodology above.

Appendix C: The Athena Framework, J.C.S. Long

The "Athena Framework": Solving the World-wide Climate and Energy Problem

Jane C. S. Long

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48. UCRL-CONF-216047

INTRODUCTION:

The energy systems we have enjoyed for the last 100 years has resulted in the advanced standard of living in the developed world and a major emerging problem with climate change. Now we face a simultaneous realization that our reliance on fossil fuels is a source of conflict and economic disruption as well as causing potentially catastrophic global climate change. It is time to give serious thought to how to collectively solve this problem. Collective action is critical since individual effort by one or only a few nations cannot adequately address the issue.

The climate and energy problem is perhaps the greatest challenge ever faced by mankind. Fossil fuel remains the least expensive and most available source of energy and the basis of our economy. The use of fossil fuels, especially over the last 100 years has led to a 30% increase in CO₂ in the atmosphere and observable global warming. The problem is growing. The population of the Earth will increase by several billion people in the next 50 years. If economic growth is to continue, the demand for energy is estimated to approximately double in the next 50 years so that we will need approximately 10 TW more energy than the 15 TW we use now. Much of this demand will come from the developing world where most of the population growth will occur and where advanced energy technology is not generally used.

The problem affects and is affected by a complex system of systems. The climate and energy problem will affect resources, social structure and the probability of increased conflict. It is the first time that the actions of each and every individual on Earth affect everyone else -- where the choice to drive an SUV in the U.S. affects the availability of water in the Himalayas, where building massive amounts of coal-fired power plants in China will cause flooding in Bangladesh and drought in California. This problem connects all the people of the world like no other problem has before. No one person, no one nation, no one technology can solve the problem. There is no parallel precedent on which to model a solution. We need a major worldwide effort on a scale never before attempted. The future of life on Earth may well depend on the outcome.

Near the end of World War II, an elite group of scientists retreated to the hills of New Mexico to develop the atomic bomb in response to a clear and present danger. The Manhattan Project gathered the best minds to put intense effort into a solution. It is no wonder that the phrase “We need a Manhattan Project for energy” is increasingly seen in commentary. The “Manhattan Project” concept is used to invoke the need for an all-out, focused effort on solving an urgent problem to a clear and present danger. In this regard, a “Manhattan Project is exactly what we need.

However, there are aspects of the Manhattan Project that are antithetical to the solutions we will have to find for the climate and energy problem. For this problem, the solution will require unprecedented collaboration between governments, scientists and citizens. The results should be highly transparent and by no means secret. Looking back on the Manhattan Project, we realize that it released a terrible new force on the world with great potential for evil. We cannot afford such a mixed outcome for climate. In fact, the solution is international and not even a “project” in the sense that a project has a clear scope, and beginning and an end. The solution in this case will be a long-term continuous effort over many years.

So, what should we call this effort to solve the most critical problem the world faces today? We propose the “Athena Framework” as a working name. Athena was a goddess of wisdom and strategy, both badly needed in this effort. She was also a warrior and by using her name we invoke a battle for life – as we know it -- on Earth. Whether this name sticks or another is chosen, the point is that the effort needs the identity of a name to help to draw people to the solution.

Fundamentally solving the climate and energy problem is a matter of societal choice. Do we continue business as usual, or do we make rational decisions that increase the likelihood of survival? We need a “framework” for making these decisions. We need to base these decisions on the best possible understanding of the systems we are dealing with. We need to realize that no matter what we do now, there will be significant and harmful outcomes from climate change already underway. We need to develop a strategy for anticipating and responding to these changes. As we look to stop this downward spiral, there are many solutions, each of which cuts a wedge into the problem and none of which can solve the problems on their own. However, each stab at the problem connects to many other issues. Nuclear power creates no greenhouse gasses, but produces radioactive waste. Hydrogen fueled cars do not emit greenhouse gases, but the production of hydrogen from fossil fuel does. The use of fossil fuel has created the enormous economic wealth in the developed world and as well created tremendous threats to security with two-thirds of the known oil supplies in the Middle East. China plans to increase power production by 1000MW per week largely with coal-fired plants and India plans a similar if smaller campaign. Solving the climate problem requires solving the problem in China and India, not just in the industrialized West. Without addressing climate change technology in the context of security, resilience, economics and development, solutions are unlikely to be realistic. A framework is needed to examine the choices in light of its connections to other issues and unintended consequences.

What does the Athena Framework look like? What does the world have to do to solve these problems? We need to examine the key actors and the key tasks. The actors are:

Society: We face a tremendous dearth of scientific literacy that would allow citizens to evaluate scientific information adequately and permit citizens to act responsibly. It is fundamentally a series of societal choices that will decide the outcome of climate change. We face the challenge to inform those choices in this country where scientific literacy is declining and declining numbers of our students choose to study science and engineering. As society does a better job of understanding the causes and effects of climate change, they can drive better policy.

Policy makers: Policy makers can create incentives, regulations and agreements that are critical to driving change in our energy systems. James Schlesinger remarked in 1989 that the U.S. has two approaches to energy policy, complacency or panic. How can we find the middle ground of rational decision-making? It is hard to even get stakeholders to the table as many are unwilling to even enter the conversation about what to do because they fear consequences of dealing with the problem are dire. People don't agree about what the problem is, never mind the solution. Also at the heart of the problem is the need for a global solution and the lack of any global institution capable of affecting a solution. If the developing world is further disadvantaged by our energy choices, global conflict will increase. In this environment policy makers must be urged to take a long-view and to find ways of dealing with complex issues without oversimplification. The long-view has a time scale of history, not the election cycle.

Scientists and engineers: Technology can help us to understand, prepare and advance but scientists must find ways to overcome institutional barriers to important collaborations and must be urged out of "admiring the problem" as opposed to solving it. They need to do a better job educating the public about their results and taking cues from policy makers about their needs. Scientists need to learn to communicate risks appropriately and engineers need to understand how technology moves from the lab to deployment.

Industry: Businesses will recognize the need for sustainable practice because they are responding to regulation or because they see it as an economic prerequisite for staying in business. In addition, they will be driven by societal values and they will drive policy to be uniform and predictable in order to control their business environment. These are all forces for the good. To be part of the solution, some businesses will have to be urged to abandon the "bunker mentality" of reacting to change as beleaguered and injured parties.

Each of these actors has a role in solving the problem. There are essentially three tasks the world must undertake:

1. **Understand the problem and predict outcomes:** It is the interaction of human behavior with the Earth's natural system that is at the heart of the climate and energy problem. We need to develop the scientific basis and capacity to understand how the natural system will behave in concert with human activity. How will temperature rise and what in turn will the temperature rise cause?
2. **Evaluate risks and adapt:** We need to have the foresight to prepare for and adapt to changes in our environment due global climate change. What changes can we expect and how shall we mitigate their negative effects? What actions should we take as insurance against probable dangers?
3. **Develop a clean energy system for the world:** Finally we must solve this problem by developing energy technologies that do not cause global climate change and are as well not a threat to security or economic well-being. Analysis shows that no one technology will solve all the problems. We need a portfolio of solutions that will allow us to provide clean energy to all peoples of the world.

Each of these three tasks is tabulated below. For each task, we discuss the reason there is an issue (“why”) and “what” might be done. Comments in the third column relate to the U.S. national program, and finally the last column provides comments applicable to the L20 Energy Security Workshop.

Task 1 Understand the climate system in order to inform policy

Why	What	Comments	L20 Energy Security Workshop
<p>Climate models: We cannot accurately predict the effect of future emissions on climate. We have no sophisticated models that can predict abrupt climate change as has been observed in the observational record. As abrupt climate change is a possibility, we need to understand how it could happen and with what certainty and impact.</p>	<p>Need research bio-geochemical cycles including carbon cycle Need regional-scale resolution and physics Need research to create such models and attempt validate against paleodata</p>	<p>Can be covered by CCSP if funded</p>	<p>This is a clear area where L20 nations can cooperate</p>
<p>Data: Our ability to understand what has happened in the past and what might happen in the future is inexorably linked to having uninterrupted and ubiquitous data of many types that can be cross-evaluated.</p>	<p>Create a national and international commitment to continuous data collection. Expand sampling, archiving and remote sensing as well as analysis and data-base management</p>	<p>Also potentially covered in CCSP. Needs funding commitment</p>	<p>This is a clear area where L20 nations can cooperate</p>
<p>Education: Most likely the tipping point on public opinion about climate change is near. But even if we begin to act now, we will not see progress on climate change for many generations. How will we insure that future generations maintain the societal will and discipline required for a long-term solution?</p>	<p>Need to develop educational curriculum and programs for K-12. Need to develop outreach programs and run public forums.</p>	<p>No program currently covers this.</p>	<p>Educational programs may be more advanced in countries such as UK where 90% of the people believe climate change and energy are problems.</p>

Task 2 Evaluate Risks and Adapt: We cannot stop climate change, how will we respond to inevitable problems?

Why	What	Comments	L20 ENERGY SECURITY WORKSHOP
<p>We will face:</p> <ul style="list-style-type: none"> ✓ Decreasing fresh water supply, frequent droughts, and increasing water demand ✓ Extreme events of deadly consequence such as heat waves, storms, floods and forest fires. ✓ Disruptions to agriculture ✓ Sea level increase, coastal erosion, melting of the permafrost ✓ Decreased pH and warming of the oceans leading to ecological damage ✓ Degraded air quality and migration of disease vectors ✓ Ecological damage due to habitat loss 	<p>To mitigate these potential risks, need a new program to facilitate adaptation, based on:</p> <ul style="list-style-type: none"> ✓ estimates of increased risk due to climate change, and their costs ✓ a wide range of technical and policy tools for dealing with the risks ✓ estimates of the cost of mitigation 	<p>We have no national coordinated program to plan and execute adaptation. Need the CCFP: Climate Change Foresight Program.</p> <p>The problems are inherently regional in nature and local impacts must be assessed and addressed. Need to develop regional programs in cooperation with the Federal program</p>	<p>Adaptation technology can be shared among countries to minimize the cost of development.</p>
<p>Impacts of climate change will be disproportionately larger in the developing world. Security threats and conflict will increase as a result.</p>	<p>Need commitments from the industrialized world to assist the developing world. Potential G8 issue?</p>	<p>Need companion bill to Hagel’s developing world technology bill to assist with adaptation.</p>	<p>L20 may be a good way to organize an international response.</p>

Task 3 Create a new energy system: The problem is huge and will require multiple approaches to solution.

Why	What	Comments	L20 Energy Security Workshop
<p>Policy: We need a much more aggressive approach to developing a new energy system. We do not understand how our current energy system works and how policy, technology and resource changes will affect the economic aspects of the system, the security of energy and the climate system</p>	<p>Build a new generation of energy models that can predict the impacts of new technology adoption, proposed policy and economic forces. Policies such as ✓ Cap and trade ✓ Efficiency standards ✓ Carbon tax ✓ Incentives ✓ Hydrogen economy must be evaluated for their effects on GHGs, economy and security</p> <p>Develop verification technology.</p>	<p>Form energy modeling consortia to develop modeling systems and address local, national and international scope issues. Carbon tax directed to support research.</p> <p>Industry will increasingly support carbon policies to establish predictable business climate & to maintain competitive position.</p>	<p>The energy system is inherently international. We need global analysis, which might be done cooperatively.</p>
<p>Efficiency: The most immediate response to our energy/climate problem is conservation and efficiency. (Goal 1 of CCTP) We need new technology to increase the use of waste energy, building efficiency technology (appliances, heating, cooling, lighting) and more efficient industrial processes and</p>	<p>✓ For cars and all products, model policy after the Japanese “ratchet” program where the leader in efficiency for each product type becomes the target for all who must meet it within 5 years. ✓ For buildings, create a pathway to energy independent buildings. Create a national rotating fund for capital to replace future operating funds. Support states to create regionally appropriate building codes similar to LEEDS.</p>	<p>All reasonable models for our future energy scenario that control GHG require a decreasing carbon intensity and greater energy efficiency. Extreme efficiency is a term of art that describes schemes to squeeze the last drop of</p>	<p>L20 countries can agree to share efficiency technology and share experience with policy.</p>

transportation.

Carbon Capture and Storage:

We will be dependent of fossil fuel for some time and need to capture and sequester carbon.. An outgrowth of GHG is the acidification of the oceans, which may lead to wide spread ecological disaster. Carbon sequestration in the form of carbonate would buffer the oceans. Other GHG must be addressed as well. (CCTP Goal 3, 4)

Energy Supply and Distribution Technology Development (CCTP goals 2,5,6) We need a whole suite of new technologies that will transform energy supply, distribution and end use eliminating GHGs and maintaining our economy and security.

SEE Table 1 for an expansion of these issues

- ✓ Require energy impact analyses as part of EIS requirements in land-use and transportation projects.
- ✓ Develop efficient and desalination and waster use technology and policy to require efficiency.

We need advances in understanding how, how much and for how long geologic C-sequestration will work.
We need efficient inexpensive capture technology
We need innovative ideas for alternative C-Sequestration and the development of carbon sequestration schemes which also provide pH buffering in the Oceans
Other GHG's such as methane are also important to control..

- Topics include:
- ✓ Renewables
 - ✓ Nuclear Power
 - ✓ Hydrogen *sans* carbon
 - ✓ Transmission
 - ✓ Distributed generation and energy storage
 - ✓ Transportation *sans* carbon
 - ✓ Transformational technology
 - ✓ Energy for the developing world

energy out of all systems.

Use existing regional cooperatives.
Industrial partnerships
The carbon capture and storage program is vastly under-funded.
Increase funding by at least an order of magnitude.

- Implementation issues include:
- ✓ Technology development
 - ✓ Technology adoption
 - ✓ Resource availability
 - ✓ Life-cycle issues

There is already an international group working on CCS.

Technology breakthroughs might be jointly developed. Nuclear power issues are inherently international because of non-proliferation and safety issues.

Table 1 Energy Supply and Distribution Technology Development

Why	What	Comments	L20 Energy Security Workshop
<p>Renewables will play a role in reducing green house gases as well as in energy security and economic development</p>	<p>Each renewable has critical issues to overcome:</p> <ul style="list-style-type: none"> ✓ Wind: land use, bird kills ✓ Geothermal: prospecting, enhancing the reservoirs, use of low temperature ✓ Biomass: non economical technology, some technology uses more energy than it gains ✓ Solar: Need to reduce the cost of solar photovoltaics from the current ~\$5,000 per kilowatt to ~\$1,000 per kilowatt. 	<p>Need programs to address critical issues that may not be supported by industry.</p> <p>Create a national RPS supported by production tax credits and game-changing research.</p> <p>Provide insurance for long-term power purchase to enable financing</p>	<p>Technology transfer will largely be through private industry</p>
<p>Nuclear Power does not produce greenhouse gases and could be an important part of climate change mitigation. The international community is moving ahead with this technology.</p>	<p>Increasing the contribution from nuclear energy will require managing the nuclear fuel cycle including nuclear waste and having safe and secure operations that are proliferation resistant.</p>	<p>Revise the U.S. nuclear power program to address systems issues in nuclear power,</p> <p>Revise Nuclear Waste Policy Act to address YMP issues</p>	<p>Requires international leadership, L20 is a likely candidate.</p>
<p>Hydrogen: The “hydrogen economy” will not contribute to the control of climate change unless we find ways to make hydrogen that do not use more energy than they produce and do not emit GHG.</p> <p>Transmission Grid failures are likely unless better power electronics can be utilized to manage the load.</p>	<p>Develop methods to obtain hydrogen fuels without releasing GHG.</p> <p>Hydrogen storage and the life of membranes in fuels cells are other issues.</p> <ul style="list-style-type: none"> ✓ Engineering design for re-engineering the grid to allow for more efficient power 	<p>Hydrogen cars do not produce GHGs, but the production of hydrogen from fossil fuel does. This is the controlling issue from a climate perspective.</p> <p>There are severe issues with transmission policy as deregulation left much of</p>	<p>Several L20 nations are considering hydrogen futures. The problems are the same.</p> <p>Countries with common borders (e.g. Canada and US) share problems.</p>

As well, it would be very helpful to be able to manage renewable intermittent power sources optimally. Superconducting grid would reduce line losses as well as allow distribution of remote renewable energy

Distributed Generation and Energy Storage:

The world is moving inexorably towards distributed generation. To the extent that the source of energy is fossil fuels, distributed energy can also mean distributed emissions where there is no hope of sequestration or control. Energy storage technology would reduce the need for peak power and make intermittent renewables more useful

Transportation:

Getting carbon emissions out of the transportation system is a major problem because we need to either have liquid fuels or develop the technology and infrastructure to use electricity. The hydrogen car is fine if the manufacturing of hydrogen for the fuel does not release GHG, or if that GHG can be sequestered.

management and reliability.
✓ Development of low-cost, superconducting transmission..

The development of distributed energy generation (DG) schemes that do not disseminate the emission of GHG or have a negative effect on health effect issues (particulates, Hg, NOx, Sox

Develop small scale, low maintenance energy storage that costs less than ~\$100 per kilowatt-hour. Energy storage in the 1 to 15 kwh range would couple to distributed renewable energy production to reduce base load fossil plant needs.

- ✓ Comparison of liquid fuels
- ✓ Liquid fuels versus electric power
- ✓ Public transportation and land-use planning

the grid without anyone responsible for maintenance and upgrade.

Typical U.S. household requires about 1 kw average power or about 24 kwh per day with peak power capability of about 10 kw. In the developing world as little as 1 kwh energy storage would be useful for small PV systems or satellite beam power. U.S. household would need 10 to 15 kwh. Advanced batteries, flywheels, small scale SMES, hot rock are candidates

Need a program focused on transportation rather than stove-piped fossil energy, hybrid cars etc. Links between stationary (electric generation) and mobile (vehicles) need to be understood.

Technology transfer likely to be through private industry.

Technology transfer likely to be through private industry.

Transformational Technology: In the long run we will need technology not available today. If we add up everything we think we have or could have with known or nearly ready technology, it isn't enough in the long term.

Fusion, space based solar, high altitude wind, sustained fusion and microwave transmission to support space based solar, methods to harness biological and genetic scientific advances for energy production

Long-term high-risk research program

L20 countries will share risk, e.g. ITER.

Developing world: The developing world will experience most of the population growth in the next 50 years and most of the growth in energy demand. The vast majority of this demand will be in India and China. Africa and South America face extreme poverty that will require energy to reverse. The vast majority of the energy sources available in the world come from coal, one of the worst sources of GHG. This problem is especially acute in the developing world.

Need international cooperation to address the environmentally acceptable use of coal. Find ways to use coal as a source of energy in environmentally acceptable ways, i.e. Without releasing GHG or other pollutants into the atmosphere. Finding energy sources for the developing world that are appropriate and environmentally benign.

Many solutions to these problems may involve integrating the energy source with the end use, such as heating, light or communications.

L20 is an important forum for cooperative solutions.